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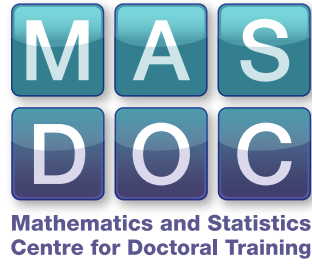
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Asymptotic Analysis and Computations of Probability Measures

by

Yulong Lu

Thesis

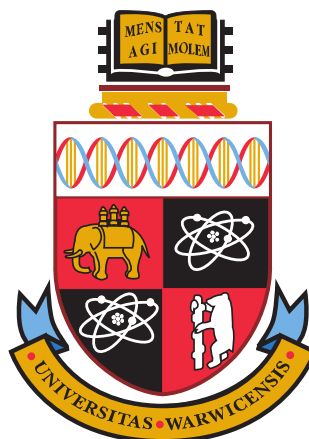
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Declarations

I declare that this thesis contains the author's original research works in collaboration with the supervisors: Andrew Stuart (Caltech), Hendrik Weber (Warwick) and Marco Iglesias (Nottingham). All the results in this thesis are completed at the University of Warwick. In particular,

(i) Chapter 1 is an introduction containing an literature review and an overview of the thesis.

(ii) Chapter 2 summarizes a few preliminary materials serving as a preparation for chapters in the sequential.

(iii) Chapter 3 is a joint work with Andrew Stuart and Hendrik Weber, and has been accepted for publication in *SIAM/ASA Journal on Uncertainty Quantification* [160].

(iv) Chapter 4 is based on the author's unpublished note and is written on the author's own. He is responsible for all proofs and calculations. Andrew Stuart and Hendrik Weber provide some insightful discussions about the mathematics and helpful comments for improving the structure.

(v) Chapter 5 is a joint work with Andrew Stuart and Hendrik Weber, and has been accepted for publication in *SIAM Journal on Mathematical Analysis* [159].

(vi) Chapter 6 is a joint work with Marco Iglesias and Andrew Stuart, which has been published in *Interfaces and Free Boundaries* [123].

Some corrections for Chapters 3, 5 and 6 were made based on the helpful comments from anonymous referees.

Abstract

This thesis is devoted to asymptotic analysis and computations of probability measures. We are concerned with the probability measures arising from two classes of problems: Bayesian inverse problems and rare events in molecular dynamics. In the former we are interested in the concentration phenomenon of the posterior measures such as posterior consistency, and the computational methods for sampling the posterior, such as the Markov Chain Monte Carlo (MCMC). In the latter we want to describe the most probable transition paths on molecular energy landscapes in the small temperature regime.

First, we examine the asymptotic normality of a general family of finite dimensional probability measures indexed by a small parameter. We begin this by studying the best Gaussian approximation to the target measure with respect to the Kullback-Leibler divergence, and then analyze the asymptotic behavior of such approximation via Γ -convergence. This abstract theory is employed to study the posterior consistency of a finite dimensional Bayesian inverse problem.

Next, we are concerned with a Bayesian inverse problem arising from barcode denoising, namely reconstructing a binary signal from finite many noisy pointwise evaluations. By choosing the prior appropriately, we show that in the small noise limit the resulting posterior concentrates on a manifold which consists of a family of parametrized binary profiles.

Furthermore, we extend the use of Gaussian approximation in the context of the (infinite dimensional) transition path problem. In particular, we characterize the most probable paths as an ensemble of paths which fluctuates within an optimal Gaussian tube. The low temperature limit of these optimal paths is also identified via the Γ -convergence of some

relevant variational problem.

Finally, we introduce, analyze and implement a novel Bayesian level set method for solving geometric inverse problems. This Bayesian approach not only removes some drawbacks of classical level set methods but also enables quantifying geometric uncertainties induced by noisy measurements.

List of Notations and Symbols

1

Function Spaces

$C(\overline{\Omega})$	Space of continuous functions on $\overline{\Omega}$.
$C^k(\overline{\Omega})$	Space of functions on $\overline{\Omega}$ with continuous derivatives up to k -th order.
$C^{0,\alpha}(\overline{\Omega})$	Space of α -Hölder continuous functions on $\overline{\Omega}$.
$BV(\Omega)$	Space of functions of bounded variations on Ω .
$L^p(\Omega)$	Space of Lebesgue measurable functions f such that $\int_{\Omega} f(x) ^p dx < \infty$.
$W^{k,p}(\Omega)$	Space of scalar Sobolev functions $f \in L^p(\Omega)$ such that the j -th derivative $D^j f \in L^p(\Omega)$ for all $1 \leq j \leq k$.
$H^k(\Omega)$	$:= W^{k,2}(\Omega)$.
$H_0^1(\Omega)$	$:= \{f \in H^1(\Omega) \mid f _{\partial\Omega} = 0\}$.
$H^k(\Omega; \mathbf{R}^d)$	Space of vector-valued Sobolev functions $\mathbf{f} = (f_1, f_2, \dots, f_d)^T \in L^2(\Omega)^d$ such that the j -th derivative $D^j f_i \in L^2(\Omega)$ for any $1 \leq i \leq d$ and $1 \leq j \leq k$.

For $(a, b) \subset \mathbf{R}$, S a finite discrete set in \mathbf{R}^d and $x_{\pm} \in \mathbf{R}^d$, we define

$$BV((a, b); S) := \{u \in BV((a, b)) \mid u(x) \in S \text{ a. e. } x \in (a, b)\}.$$

$$H_{\pm}^1(a, b) := \{u \in H^1(\Omega; \mathbf{R}^d) \mid u(a) = x_-, u(b) = x_+\}.$$

¹The list only collects few notations and symbols that are commonly used in the whole thesis. Other notations are defined in individual chapters.

Convergences

Let $f_n, f \in X$ with some Banach space X . Let F_n, F be a sequence of functionals defined on the same metric space Y . Let Z_n, Z be a sequence of random variables defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$.

$f_n \rightarrow f$	f_n converges to f strongly in X .
$f_n \rightharpoonup f$	f_n converges to f weakly in X .
$F_n \xrightarrow{\Gamma} F$	F_n Γ -converges to F .
$Z_n \rightarrow Z$ \mathbb{P} -a.s.	Z_n converges to Z \mathbb{P} -almost surely.
$Z_n \xrightarrow{\mathbb{P}} Z$	Z_n converges to Z in probability.
$Z_n \xrightarrow{d} Z$	Z_n converges to Z in distribution.

Miscellaneous Notations

\mathbb{E}^μ	The expectation with respect to the probability measure μ .
$\mu \ll \nu$	The measure μ is absolutely continuous with respect to the measure ν .
$X \sim \mu$	X is a random variable distributed according to the probability measure μ .
$a \wedge b$	The minimum value of a and b .
$a \vee b$	The maximum value of a and b .
$a \lesssim b$	$a \leq C b$ for some universal constant $C > 0$.
$a \gtrsim b$	$a \geq C b$ for some universal constant $C > 0$.
$a \simeq b$	$a \lesssim b$ and $a \gtrsim b$.
$\mathbf{1}_A$	Indicator function of the set A .
$f^* \mu$	The push-forward of the probability measure μ under a Borel-measurable map f .

Chapter 1

Introduction

1.1 Overview

Uncertainty is an intrinsic attribute of the real world. This uncertainty may come, for example, from the unpredictability of physical experiments, a lack of knowledge about physical processes or from noisy measurements. To understand and quantify the uncertainties from various sources as well as their impacts, probabilistic modelling is becoming an increasingly important methodology. For instance, statistical physicists use methods of stochastic processes to describe the thermal motion of particles at the microscopic scale, and link the stochastic microscopic properties of particles to the deterministic macroscopic behaviour of the physical system through hydrodynamic limits. Meteorologists predict the weather and climate of a given location by assimilating the real time noisy data into stochastic dynamical models that approximately describes the atmospheric processes. In many stochastic models, the central mathematical object is usually a probability measure (or distribution), which contains rich uncertainty information about the quantities of interest. It is thus highly important to think about how to learn from probability measures.

In this thesis we focus on a family of probability measures $\{\mu_\varepsilon\}_{\varepsilon>0}$ of the form

$$\mu_\varepsilon(du) = \frac{1}{Z_\varepsilon} \exp\left(-\frac{1}{\varepsilon}\Phi_\varepsilon(u)\right) \mu_0(du), \quad (1.1)$$

where ε is a small parameter, Z_ε is the normalisation constant and μ_0 is a probability measure independent of ε . Probability measures μ_ε of the form (1.1) arise naturally from a variety of applications, among which of particular interest in this thesis are Bayesian inverse problems and the transition path problem in molecular dynamics. In Bayesian inverse problems, the measure μ_ε is a posterior measure, in which the functional Φ_ε is the negative log-likelihood, the measure μ_0 comes from the prior distribution, and the parameter ε

is usually associated with the number of observations or the noise level of the statistical experiment. In this case, the formula (1.1) is nothing but the Bayes' formula. Whereas in the transition path problem, the measures μ_ε and μ_0 are the distribution of certain (conditioned) diffusion process and that of the underline Brownian bridge process respectively, and the parameter ε is proportional to the physical temperature. In this case, the formula (1.1) follows from the Girsanov transformation.

This thesis studies the probability measures μ_ε from both theoretical and computational perspectives. From a theoretical point of view, we are interested in understanding the asymptotic behaviour of probability measures μ_ε in the limit $\varepsilon \downarrow 0$. The primary motivation for this theoretical study comes from the issue of *posterior consistency* for Bayesian inverse problems. Posterior consistency refers to the property that if the data is generated from some “true” parameter then the updated posterior measures concentrate around the truth as the information of the data grows up to infinity. This consistency property is important since it guarantees that Bayesian inferences with different priors will agree as long as the data is sufficiently informative. Another motivation comes from the analysis of transition paths in molecular dynamics, where we would like to give an efficient description of typical transition paths at finite temperature as well as the limiting behaviour of such paths in the low temperature limit. From a computational point of view, we would like to extract useful information from a measure μ_ε (with a fixed ε). One common approach for doing so is to draw samples from a probability measure by using Markov Chain Monte Carlo (MCMC) methods. MCMC methods are of great importance since they are the only computational tool that could provide complete information about a probability measure. We will implement a MCMC algorithm within a Bayesian level set method for solving geometric inverse problems. Nevertheless, direct MCMC simulations can be prohibitively expensive in general. As an alternative, point estimators, such as the expected value and the maximum a posteriori (MAP) estimator are commonly used in practice owing to their computational tractability. The downside of point estimators lies in the fact that they lose the uncertainty information of the measure. In this thesis, we seek a good compromise between point estimators and MCMC methods via Gaussian approximations. We shall demonstrate the power of the Gaussian approximation approach in the theoretical studies of Bayesian inverse problems and the transition path problem.

The rest of this chapter is organised as follows. Section 1.2 and Section 1.3 provide an overview of the Bayesian inverse problems and rare events in molecular dynamics respectively, with emphasis on the theoretical and computational issues therein. In Section 1.4, we discuss two principle ingredients used in the thesis for analysing the asymptotic behaviour of probability measures: Gaussian approximations and Γ -convergence.

1.2 Bayesian Inverse Problems

Inverse problems concern converting observational data into information about systems which are not observed directly. From the mathematical point of view, an inverse problem takes the abstract form

$$y = \mathcal{G}(u)$$

in which the unknown $u \in U$ is to be determined, given the data $y \in Y$, where U and Y are Banach spaces. The operator $\mathcal{G} : U \rightarrow Y$ is usually termed as the *forward operator* and in general it is written as the composition of a *solution operator* coming from the forward model and an *observational operator*. Most inverse problems of interest are often ill-posed in the Hadamard sense: they might not have a solution in the strict sense, solutions might not be unique and/or might not depend on the data continuously. The last scenario arises, in particular, when we have noisy observations such as

$$y = \mathcal{G}(u) + \eta$$

where η is an additive noise. In classical approaches to inverse problems, the noise is treated deterministically although it may be modelled in terms of a probability distribution and the inverse problem is solved through minimising the data-misfit functional. The ill-posedness of the inverse problem is reduced by means of regularisation techniques, such as the Tikhonov regularisation [219]. In the present thesis we will not consider classical approaches to inverse problems, but we refer the reader to the monographs [87, 132] for extensive treatments of optimisation-based regularisation methods.

We focus on a statistical approach to inverse problems, in which all quantities including the unknown u , the noise η and the observations y are regarded as random variables. The Bayesian approach updates the knowledge about the unknown by blending prior beliefs with observed data. Mathematically, the prior belief is encoded in a *prior distribution* μ_0 on the unknown. The probabilistic information of the noise is useful in defining the data likelihood, that is the conditional distribution of y given u , describing the possibility of observing certain outcome given a fixed unknown parameter. Bayes' rule combines the prior distribution and the data likelihood, leading to a probability measure called the *posterior* μ^y , that is the conditional distribution u given y . Typically the Bayes' rule implies that the posterior measure is absolutely continuous with respect to the prior and has the Radon-Nikodym derivative

$$\frac{d\mu^y}{d\mu_0}(u) \propto \exp(-\Phi(u; y)).$$

This exponential form arises in particular when the noise distribution is Gaussian and in this case the functional $\Phi(u; y)$ admits a form of least square. The Bayesian approach offers the following advantages over classical regularisation approach:

(i) The posterior measure is the solution to the Bayesian inverse problem, from which one can not only estimate the unknown under consideration but also quantify the uncertainty about the unknown. Uncertainty quantification (UQ) plays an important role in characterising the impact of variability and lack-of-knowledge about the quantify of interest.

(ii) The maximum a posterior (MAP) estimator, a point u maximising the posterior density function μ^y in the Bayesian approach, is linked with the minimiser of some regularised functional, in which the regularisation norm arises naturally from the prior.

(iii) Bayesian inverse problems are usually well-posed with respect to the data, that is the posterior measure μ^y depends continuously on y ; whereas the solutions to classical inverse problems are very sensitive to the data y .

The book [136] is a good reference including an introduction to Bayesian inverse problems and some applications in science and engineering. The problems considered there come from infinite dimensional models such as partial differential equations (PDEs), but the Bayesian inferences are carried out only for discretised problems which are therefore essentially finite dimensional. A modern treatment of infinite dimensional Bayesian inverse problems can be found in the excellent review articles [215] and [61]. The paper [63] gives a definition of MAP estimators in the infinite dimensional setting based on the idea of maximising the ratio of two small ball probabilities, and the close relationship between MAP estimators and regularisation methods is explored as well therein.

1.2.1 Issues and Challenges

The Bayesian approach eliminates or reduces the ill-posedness of inverse problems by searching the solution in a larger space – the space of probability distributions instead of the space of deterministic states. As discussed earlier, the probabilistic formulation brings several benefits, but it also brings some issues and challenges as we elaborate below.

1.2.1.1 Choice of Priors

The Bayesian approach provides a natural regularisation by means of introducing a prior distribution. The prior represents all possible information about the unknown quantity that one may have prior to observations, hence it should be tailored according to the specific structure and property of unknowns. For example, in the modelling of discontinuous permeability of the subsurface, Gaussian priors may not be appropriate since geological perme-

ability usually exhibits some heterogeneous structures such as layers and channels. In practice, the quantity of interests may also involve different scales of length and amplitude, for which Bayesian inferences can be very sensitive to the length scales in the priors. For those problems, modelling priors hierarchically, through the introduction of hyper-parameters and hyper-priors, is helpful for improving the robustness of estimation. In general, the choice of prior is still subjective, and how to choose priors to increase the accuracy and efficiency of Bayesian inferences has become one of the biggest challenges.

Gaussian priors [61, 215] are the most commonly used priors in Bayesian inverse problems of functions, since they are easy to construct and the parameters thereof are directly linked to the regularity of functions. Besov priors [62, 143] are useful in imaging problems where preserving the edges and interfaces is important. The book [136] provides an overview of different priors used in statistical inverse problems in the finite dimensional setting. Applications of hierarchical models in inverse problems can be found for example in [42, 73, 118]. In particular, in [118] a hierarchical Gaussian prior was used in linear Bayesian inverse problems and the MAP estimator of the resulting posterior was connected with the Mumford-Shah functional. In [73], hierarchical priors based on the Whittle-Matérn distributions were used in a Bayesian level set framework for controlling length scales in geometric inversions.

In this thesis, we will show how to construct prior models in the context of barcode denoising (Chapter 4) and geometry inversion (Chapter 6).

1.2.1.2 Asymptotic performance

The quality of Bayesian procedures can be assessed by the asymptotic performance of the posterior measure. It is desirable that as more and more samples are generated from some *true* model, the posterior based on these samples would concentrate around the truth. This property is formally phrased as *posterior consistency*. Let us give it a precise definition in the context of Bayesian inverse problems. Consider the inverse problem of recovering the true parameter u^\dagger from a sequence of observations

$$y_j = \mathcal{G}(u^\dagger) + \eta_j.$$

Let μ_n be the posterior measure built upon the accumulated data $Y_n := \{y_j\}_{j=1}^n$ and E^{Y_n} be the expectation with respect to the law of Y_n . We say that the posterior μ_n is consistent at u^\dagger if for any $\delta > 0$

$$\mathbb{E}^{Y_n} \mu_n \{u \mid d(u, u^\dagger) \geq \delta\} \rightarrow 0 \text{ as } n \rightarrow \infty. \quad (1.2)$$

Here d represents a metric on the parameter space. In addition, we say that the posterior is consistent with contraction rate ε_n with $\varepsilon_n \rightarrow 0$ if

$$\mathbb{E}^{Y_n} \mu_n \{u \mid d(u, u^\dagger) \geq M_n \varepsilon_n\} \rightarrow 0$$

for every $M_n \rightarrow \infty$ as $n \rightarrow \infty$.

In Bayesian statistics, the famous Doob's consistency theorem [65, 69] shows that under certain mild assumption on the prior the posterior measure is consistent for almost every true parameter, but it does not give consistency at a given truth. Schwartz' theorem [208] allows proving consistency in the weak sense under the conditions that the true distribution fulfils certain testability property and that any small neighbourhood (measured in terms of the Kullback-Leibler divergence) of the true distribution has positive probability under the prior. The papers [13, 102] improved the weak convergence in the Schwartz' theorem to strong convergence. Posterior contraction rates were also obtained for non-parametric statistical models; see e.g. [103, 105, 210]. In the context of Bayesian inverse problems, the contraction rates were studied mostly for linear inverse problems with Gaussian priors; see [2, 140] for the mildly ill-posed case and [3, 141] for the severely ill-posed case. The paper [195] proved a contraction result for linear inverse problems with non-conjugate priors. The papers [176, 192] investigated the posterior contraction rate in the problem of Bayesian nonparametric drift estimation of SDEs. For nonlinear Bayesian inverse problems, the posterior contraction results are quite limited. The paper [224] focused on the contraction rate for a specific nonlinear infinite dimensional Bayesian inverse problems arising from groundwater flow modelling. For a good review of posterior consistency we refer the reader to [101].

In many statistical problems, the concentration phenomenon of posterior consistency can be characterised even more precisely. The famous Bernstein-von Mises (BvM) theorem states that under certain conditions the posterior measure is asymptotically equivalent to a Gaussian distribution independently of the prior when the sample size is sufficiently large. Let us consider the BvM theorem more precisely in a parametric setting. Suppose that $\mathbf{X}^N := \{X^1, X^2, \dots, X^N\}$ are a collection of independent and identically distributed (i.i.d) samples with each X^i drawn from a distribution P_θ . We also assume that the parameter $\theta \in \Theta$. Let P_θ^N be the law of \mathbf{X}^N . Let Π be the prior distribution on Θ and denote by $\Pi(\cdot | \mathbf{X}^N)$ the resulting posterior distribution. The Bernstein-Von Mises Theorem states that under the frequentist assumption that X^i is drawn from some true model P_{θ_0} , as $N \rightarrow \infty$

$$d_{TV} \left(\Pi(\theta | \mathbf{X}^N), N \left(\hat{\theta}_N, \frac{1}{N} I_{\theta_0}^{-1} \right) \right) \xrightarrow{P_{\theta_0}^N} 0, \quad (1.3)$$

where $\hat{\theta}_N$ is an efficient estimator for θ , I_θ is the Fisher information matrix of P_θ and d_{TV} represents the total variation distance. The BvM theorem is important at least in two ways. First, a direct consequence of the BvM result (1.3) is that the posterior contracts around the truth with the rate $\mathcal{O}(N^{-1/2})$. Second, the BvM result implies that Bayesian credible sets are asymptotically equivalent to frequentist confidence intervals, whereby the estimation of the latter can be realised by making use of the computational power of MCMC algorithms.

The BvM theorem for parametric models is well-known, see for example [43, 65, 121]. Semiparametric versions of BvM phenomenon, concerning the asymptotics of the marginal posterior distribution for a finite dimensional parameter of interest from a model of infinite-dimensional nuisance parameter, have been shown to be valid in various occasions [18, 48, 209]. For statistical models with infinite parameters (usually rephrased as nonparametric models), the BvM theorem does not hold in general. Some counterexamples can be found in [59] and [97]. Although BvM results in strong L^2 -setting are not available in nonparametric models, it is possible to prove some weak versions of BvM, see e.g. [46, 47, 145]. In [46], the author proved a nonparametric BvM theorem under weak L^∞ -topology in the Gaussian white noise model. This result was extended to the i.i.d sampling model in [47]. The recent book [106] provides a detailed review of semiparametric and nonparametric BvM results.

It is important to notice that posterior consistency does not hold in any Bayesian inference for under-determined inverse problems since the data can not determine the unknown uniquely. For those problems, posterior measures can only be expected to concentrate on manifolds in general. We will show this type of concentration in both Chapter 3 and Chapter 4.

1.2.1.3 Computation

The most important step of Bayesian inferences is to extract useful information from posterior distributions. The most widely used approach is to sample from posterior distributions by using Markov Chain Monte Carlo methods. The resulting samples are then used to compute quantities of interest, such as the expectation of observables. The key idea of MCMC is to design a suitable Markov chain so that its stationary distribution coincides with the target posterior measure. A standard Metropolis-Hastings [117, 168] based MCMC algorithm is given in Algorithm 1.2.1.

Algorithm 1.2.1 (Metropolis-Hastings Algorithm). *Given a target measure μ on \mathbf{R}^d with density π and a transition kernel p , samples $\{x_k\}$ are generated in the following steps.*

1. *Initialisation: set $k = 0$ and pick $x_0 \in \mathbf{R}^d$.*

2. *Propose* $y_k \sim p(x_k, \cdot)$.
3. *Set* $x_{k+1} = y_k$ *with probability*

$$a(x_k, y_k) := \min \left\{ 1, \frac{\pi(y_k)p(y_k, x_k)}{\pi(x_k)p(x_k, y_k)} \right\}.$$

4. *Set* $x_{k+1} = x_k$ *otherwise.*
5. $k \rightarrow k + 1$ *and return to 2. .*

A great advantage of MCMC is that it only requires specifying the target measure up to a normalisation constant; this can be seen from the ratio in Step 3 of above. Different choices of transition kernel p gives MCMC algorithms of different types and degrees of efficiency. There exists a vast literature concerning the theory, implementation and application of various MCMC methods; see relevant discussions in excellent textbooks [152, 197, 200]. Applications of MCMC in Bayesian inverse problems can be found in [136]. One of the biggest challenges of MCMC is that its computational complexity usually increases dramatically with the number of dimensions. The optimal complexity as a function of dimension of the state space has been identified in many MCMC algorithms, see e.g. [100, 165, 185, 198, 199]. In particular, with an appropriate scaling of the proposal variance according to the dimension, the resulting Markov chain converges to a stochastic (partial) differential equation. The understanding the diffusion limits of MCMC in high dimensions has facilitated the development of MCMC algorithms for functions, including the preconditioned Crank-Nicolson MCMC (pCN-MCMC) method [57, 111] and hybrid Monte Carlo (HMC) method [57, 181]. Sequential Monte Carlo (SMC) [72, 172], based on the evolution of interacting particles is another popular sampling method used in practice. SMC is also known as particle filter [144, 162] in the community of data assimilation and has been proved to be very efficient in low dimensions, but has poor performance in high dimensions [16]. Recently, dimension-independent versions of SMC were proposed and applied for solving inverse problems in [17, 137].

For high-dimensional problems, full characterisations of the posterior distributions can be very difficult. In this case, it is convenient to use some point estimators instead. Posterior means and MAP estimators are commonly used “typical” values from posterior distributions. In Bayesian inverse problems, the MAP estimator is of great interest since it directly links to classical regularisations [63, 118]. Recently, a stochastic Newton algorithm was proposed in [133], where a local Gaussian approximation around the MAP estimator was used in the construction of the proposal in MCMC in order to improve the efficiency of vanilla MCMC algorithms. A similar Gaussian approximation idea was exploited for accelerating the pCN-MCMC algorithm in [190].

1.2.2 Geometric Inverse Problems

Geometric inverse problems are a special class of inverse problems where the unknowns are geometric shapes. Typical geometric inverse problems include seismic inversion and reservoir characterisation [20, 128], inverse scattering problems [56, 109, 139], electrical impedance tomography [23, 52], etc. In the resolution of geometric inverse problems, the mathematical modelling of the shapes is a key preliminary step. The level set method, initially proposed by Osher and Sethian [179], provides an advantageous tool for representing and analysing surfaces and interfaces over standard parametric models. Since the paper by Santosa [204], level-set-based shape optimisation methods have been successfully applied to various geometric inverse problems, see e.g. [5, 35, 36, 55, 128]. As pointed out in [37], despite the popularity of level-set-based optimisation methods, their mathematical analysis turns out to be a very difficult matter. In particular, the convergence of the optimisation algorithms is only known in few circumstances [35, 36] and the regularity of level sets during the evolution defined by the optimisation procedure still remains an open problem. These theoretical issues are mostly due to the occurrence of discontinuity in the level set representation. More precisely, the mapping that takes a level set function to the physical parameter space is discontinuous. The discontinuity also causes troubles in the numerical implementation of level set methods. For instance, standard level set methods tend to produce more and more flat level set functions during the evolution, see [37, 91]. Hence some ad hoc reinitialisation operations need to be performed periodically in practice to reinstate the geometric motion. Some of these negative aspects of conventional level set methods can be eliminated by a novel Bayesian level set method [123] which we will discuss in Chapter 6. A hierarchical version of the Bayesian level set method is presented recently in [73].

1.3 Rare Events in Molecular Dynamics

Understanding transition events in complex and dynamical molecular systems is fundamental to the understanding of many processes in physics, biochemistry and material sciences. Often, transition processes of interest are “rare” in the sense that the system of consideration spends a long period of time fluctuating around the neighbourhood of the so-called metastable states before it “rarely” hops from one metastable state to another. Protein folding — the most fundamental processes of biological self-assembly, is a typical example of such rare events. Uncovering the mechanism of protein misfolding and aggregation could possibly help to prevent or cure a wide range of human diseases; see e.g. [67, 68]. In the process of protein folding, the transition from an unfolded state to a final native state is usually on the timescale of microseconds to seconds, whilst the timescale of the vibration of covalent bonds is only femtoseconds.

Understanding the detailed behaviour of transition paths of a molecule system often requires calculations of multiple trajectories. Direct simulations of the trajectories, or solving the underlying stochastic differential equations (like equation (1.5) below), is computationally hindered by a number of challenging issues, including high dimensionality [207], dilemma of stability and time-step [146, 147], wide disparity of timescales [79, 220], etc. Hence it becomes essential to seek alternative effective descriptions of dynamical systems. Below we will give a brief overview of the analysis and computations of rare events in that direction. Before that we want to first present a paradigmatic model — the Langevin dynamics model for the study of rare events in molecular dynamics.

1.3.1 Langevin Dynamics Model

In molecular dynamics, the thermal-driven movements of a system of molecules and atoms can be modelled in terms of Newton mechanics, where the interaction forces between individual atoms are derived from the gradients of a potential energy function (or energy landscape), which describes the internal potential energy of bonded or non bonded interactions between atoms. Perhaps the most popular mathematical model of molecular dynamics is the so-called Langevin dynamics [146, 148]

$$\begin{aligned}\frac{dx}{dt} &= -\mathbf{M}^{-1}p, \\ \frac{dp}{dt} &= -\nabla V(x) - \gamma \cdot p + \sqrt{2\gamma k_B T} \mathbf{M}^{1/2} \frac{dW}{dt}.\end{aligned}\tag{1.4}$$

In the above model, \mathbf{M} is the mass matrix and V represents the potential energy function. The parameter γ is referred to as the friction coefficient or collision rate, which is assumed to be a universal constant here, but can be generalised to be a spatial-dependent tensor. The constant k_B is the Boltzmann constant, T is the physical temperature and W stands for a standard Brownian motion so that \dot{W} gives the standard Gaussian white noise, which models the effects of the heat bath.

A simplified but still widely used version of the Langevin dynamics is the Brownian dynamics

$$\frac{dx}{dt} = -\nabla V(x) + \sqrt{2\varepsilon} \frac{dW}{dt}.\tag{1.5}$$

The Brownian dynamics can be derived from the Langevin dynamics by taking the limit of large friction or small mass (see [148] for explicit derivations). For this reason, the Brownian dynamics is also called the *overdamped Langevin dynamics*. We note that the parameter ε is a constant determined in the limit and in particular it is proportional to the temperature. Under some mild conditions [201] on the potential V , the Brownian dynamics

defines a reversible Markov process with invariant measure

$$\rho_\varepsilon(dx) \propto \exp\left(-\frac{1}{\varepsilon}V(x)\right) dx.$$

The phenomenon of metastability is illustrated in Figure 1.1, which shows a trajectory for a Brownian particle moving in a double-well potential.

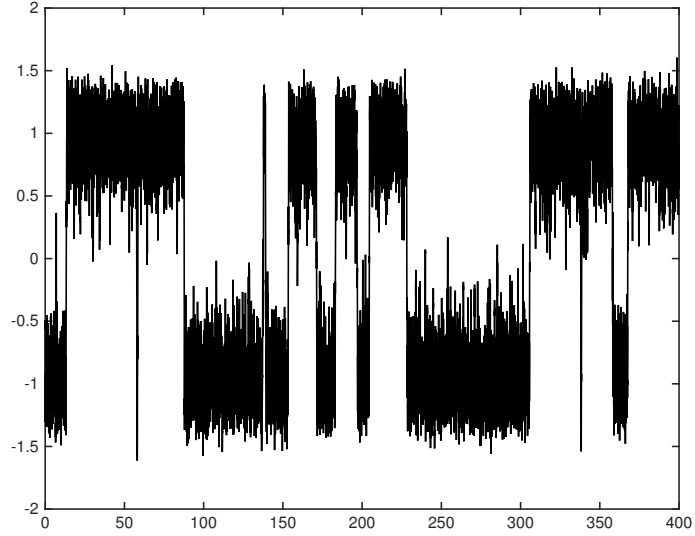


Figure 1.1: Brownian dynamics with double well potential $V(x) = \frac{1}{4}(x^2 - 1)^2$ and noise level $\varepsilon = 0.6$.

1.3.2 Rare Events Analysis

The transition state theory (TST), developed by Arrhenius [9], Eyring [93], M.G. Evans and M. Polanyi [92], et al, provides a primary framework to study qualitative behaviour of rare events in dynamical systems. The theory is focused on the identification of the transition states and the calculation of the associated transition rates. Transition states are the bottlenecks for rare events and usually correspond to the saddles of the underlying potential energy landscape. The transition rate describes the frequency of each transition, and can be calculated from the probability flux of reactive trajectories passing through the neighbourhood of the transition state. To give an example, consider the one dimensional over-damped Langevin dynamics with a double well potential V , i.e. V has two local minimisers x and y , separated by a unique saddle point z . According to Arrhenius law [9],

the transition rate from x to y is given by

$$\kappa_{A \rightarrow B} \simeq C e^{[V(z) - V(x)]/\varepsilon} (1 + o(1))_{\varepsilon \downarrow 0}.$$

The prefactor C can be calculated explicitly by Eyring-Kramer’s formula [15, 142] and it depends only on the curvatures of V at x and z . Disregarding the prefactor, the exponential asymptotics can also be derived from large deviation principle [98].

From a mathematical point of view, TST implies that a transition process can be reduced to a finite state continuous time Markov chain, with the state spaces defined by the metastable states and the jump probabilities given by the transition rates. The metastability property of the original dynamics can be understood by that of the finite-state Markov chain; see e.g. [24, 178].

The idea of TST has a far-reaching influence on the development of rare events in both theories and computations. The well-know transition path sampling (TPS) method developed by Bolhuis, Chandler, Dellago and Geissler [182] is based on (and goes beyond) TST and allows generating reactive trajectories between two stable states using MCMC algorithms. From the ensembles of reactive trajectories, one could in principle retrieve some dynamical information about the reaction mechanism, such as the reaction rate, reaction coordinate, etc. However, the process of doing so is highly non-trivial (see e.g. [173]). Therefore it is necessary to have new approaches to interpreting the reactive trajectories. The transition path theory (TPT) [84, 220] provides a new mathematical framework for understanding the statistical properties of the transition paths between two states. In TST, a transition path from state A to state B is defined as the piece of reactive trajectory from A to B without going back. Different from TPS, the length of the reactive trajectories is not fixed any more and could possibly be infinite. The most important feature of TST is that it allows to analyse and to compute many interesting statistical quantities of the transition path ensemble, such as the likelihood of finding a reactive trajectory at any spatial point (or probability density of reactive trajectory and currents) and the reaction rate (or the probability flux). For more discussions on TST, we refer to [79, 156, 169] and the references therein.

1.3.3 Rare Events Computations

Over the last two decades, significant progress has been made in developing different numerical techniques for rare events computations. We intend to give a brief overview of several different types of numerical methods according to different quantities one might want to estimate.

First in the small temperature regime, the occurrence of transition events can be

predicted with high probability by the so-called minimal energy paths (MEPs). Roughly speaking the probability of visiting the neighbourhood of other paths rather than the MEPs is exponentially smaller. A complete analytical characterisation of this picture is due to the well-known theory of Freidlin-Wentzell [98] based on the large deviation principle. Building upon the Freidlin-Wentzell theory, many algorithms have been proposed for finding the minimal energy paths. Notable methods include the nudged elastic band method [135], the string method [80, 82, 83], minimal action methods [81, 234] and geometric minimal action methods [108, 120, 221].

At finite temperature, the transition paths sampling [182] is perhaps the first systematic numerical method for generating the ensemble of transition pathways between two metastable states. Traditional random walk based MCMC algorithms are often too slow to be used in practice, hence many techniques have been developed to improve the efficiency of sampling from different perspectives. Hyperdynamics, developed by Voter [225], accelerates escaping from stable states of the dynamics by modifying the potential energy near those states. This biased potential of course changes the transition time, but the statistics of the original system can be recovered by an appropriate time rescaling. The similar idea is extended to temperature-accelerated dynamics [211] method whereas the exit event is speed up by increasing the temperature rather than potential biasing. Replica exchange sampling [217, 226], also known as parallel tempering [85, 216], improves sampling efficiency through a swap mechanism that exchanges replicas of the system of different temperatures or different potentials [157, 232]. It has been observed that the efficiency of replica exchange sampling methods increases as the swapping frequency tends to infinity [75, 191].

Importance sampling is an important class of methods for rare events simulation. It is particularly useful to compute the expectation of observables under the distribution of transition paths, such as the exit probability and the free energy. The key idea of importance sampling is to draw samples from a different distribution so that on the one hand the samplers could explore important regions more frequently, and on the other hand to decrease the variance of statistical estimation. How to choose the alternative distribution to achieve variance reduction is a central issue. Dupuis et al. established a framework [76, 77] based on large deviation theory [74] and optimal control theory [95] to analyse the efficiency of importance sampling. The theoretical analysis leads to a series of asymptotic *optimal* importance sampling methods [114–116, 222, 233] in the sense that the relative statistical error is uniformly bounded or vanishing.

1.4 Two Ingredients: Gaussian Approximation and Γ -convergence

The idea of approximating a (non-Gaussian) probability measure by a Gaussian measure or a mixture of Gaussians is essential in a variety of applications. For example, in machine learning Gaussian mixture distributions [19] are widely used for representing the probability distribution of observations which may involve subclassifications in the overall population, and hence they are of great importance in the processing of large data set, such as clustering of point clouds, image segmentation and image compression. In data assimilation [144], the Kalman filter is an exact algorithm for linear Gaussian problems (with additive Gaussian noise); for non-linear problems, most important filters, such as the extended Kalman filter (ExKF) and the ensemble Kalman Filter (EnKF) are approximate Gaussian filters [144], in which Gaussian approximations are carried out in the prediction step. Although the Gaussian approximation is extensively used in applications, it had not been treated in a substantial systematic theory until very recently. In the paper [187], the authors studied the best Gaussian approximation from a calculus of variations perspective, and more specifically they formulated a variational problem by employing the Kullback-Leibler (KL) divergence as the cost functional. Owing to some nice properties of the KL-divergence, they were able to prove the existence of minimisers to the variational problem. We will adopt the same calculus of variations viewpoint to study Gaussian approximations for probability measures in this thesis, but with more emphasis on the asymptotic behaviour of the best approximation in some small parameter limit. In particular we want to address three questions:

- (1) Does the best Gaussian approximation converge in the small parameter limit?
- (2) Does the limit of the best Gaussian satisfy a limit variational problem?
- (3) How accurate is the approximation?

To answer the above questions, we employ a key mathematical tool — Γ -convergence [25, 164]. In the field of calculus of variations, Γ -convergence is an important notion for studying convergence of functionals and has been widely used in solving asymptotic problems in mathematics and physics; see for example [12, 96, 171, 189]. In our study of Gaussian approximations, we prove the Γ -convergence of some functionals that are closely associated to the KL-divergence between the target measure and the Gaussian measures. Identifying the Γ -limit provides a direct answer to question (2). If in addition the sequence of functionals fulfils certain compactness property, then Γ -convergence of the functionals guarantees the convergence of minimisers and minimum values; this gives answers to question (1) and (3). The established Gaussian approximation theory is exemplified in the analysis of Bayesian inverse problems and the transition path problem. More specifically, in Chapter 3 we study the posterior consistency of a finite dimensional and nonlinear Bayesian inverse problem and in particular we prove a Bernstein-von Mises theorem for the posterior

measure. In Chapter 5 we use the best Gaussian approximation to characterise the optimal Gaussian tube around the most likely transition paths.

1.5 Outline of Contributions

In this thesis, we discuss the asymptotic behaviour of probability measures arising from two classes of problems: Bayesian inverse problems (Chapter 3 and Chapter 4) and the transition path problem (Chapter 5). In Chapter 6, we focus on the computational aspects of probability measures in the study of a Bayesian level set method for geometric inverse problems. Below we give an outline of each chapter.

1.5.1 Chapter 3 – Gaussian Approximations for Probability Measures on \mathbb{R}^d

This chapter concerns the approximation of probability measures on \mathbb{R}^d with respect to the Kullback-Leibler divergence. We are interested in a family of probability measures $\{\mu_\varepsilon\}_{\varepsilon>0}$ where a measure μ_ε has a Lebesgue density

$$\rho_\varepsilon(x) = \frac{1}{Z_{\mu,\varepsilon}} \exp\left(-\frac{1}{\varepsilon} V_1^\varepsilon(x) - V_2(x)\right).$$

We assume that $V_1^\varepsilon \rightarrow V_1$ locally and V_1 has n distinct minimisers x^1, x^2, \dots, x^n . Intuitively, when ε is small, the measure μ_ε is a multi-modal distribution and each mode locally looks like a Gaussian measure with centre near the individual minimisers x^i and with covariance scaled like $\mathcal{O}(\varepsilon)$.

Given a measure μ_ε with a fixed positive ε , we consider the minimisation of the Kullback-Leibler divergence $D_{\text{KL}}(\nu||\mu_\varepsilon)$ with respect to ν over two classes of simple measures: Gaussian measures and Gaussian mixtures (convex combinations of Gaussian measures). The existence of the best approximation ν_ε is proved in both cases. Moreover, the asymptotic behaviour of ν_ε in the limit $\varepsilon \downarrow 0$ is characterised explicitly by studying the Γ -convergence of functionals associated to the KL-divergence $D_{\text{KL}}(\nu||\mu_\varepsilon)$. It turns out that the relative entropy structure is preserved in the Γ -limit, which consists of two parts: the first part is a weighted relative entropy which measures the discrepancy between two Gaussians, and the second part is the relative entropy between two Dirac masses supported at x^i with different weights, with one coming from the weight of the Gaussian mixture and the other from the asymptotics of the normalisation constant $Z_{\mu,\varepsilon}$ in the definition of the target measure. As a consequence of the Γ -convergence result, the best Gaussian approximation ν_ε is given by $\nu_\varepsilon = \sum_{i=1}^n \alpha_\varepsilon^i \mathcal{N}(m_\varepsilon^i, \varepsilon \Sigma_\varepsilon^i)$ with

$$m_\varepsilon^i \rightarrow x^i, \Sigma_\varepsilon^i \rightarrow D^2 V_1(x^i)^{-1}, \alpha_\varepsilon^i \rightarrow [\det D^2 V_1(x^i)]^{-\frac{1}{2}} \cdot e^{-V_2(x^i)}.$$

As a typical application of the abstract theory, we consider the finite dimensional Bayesian inverse problem of recovering x from the noisy observations y_ε , where

$$y_\varepsilon = G(x) + \varepsilon\eta.$$

Here $G : \mathbf{R}^d \mapsto \mathbf{R}^d$ is the (nonlinear) forward map and the noise $\eta \sim \mathcal{N}(0, \mathbf{I}_d)$. By imposing a suitable prior on x , we can obtain the posterior μ_ε^η . For a fixed realisation of noise, we show that the posterior measure is approximately equivalent to a Gaussian (or a Gaussian mixture) in the small noise limit; (2) Taking into account the randomness of the noise, we prove a BvM theorem (with optimal rate of convergence) for the posterior measure.

1.5.2 Chapter 4 – Bayesian Approach to Barcode Denoising

In this chapter we investigate a Bayesian approach to the recovery of a barcode signal from finitely many noisy observations. In our set-up, a barcode signal is a one-dimensional binary function u defined on the interval $[-1, 1]$ and taking values in $\{\pm 1\}$. The inverse problem is to recover u from noisy pointwise evaluations $\{f_i\}_{i=1}^N$ at sampled points $\{x_i\}_{i=1}^N \subset (-1, 1)$, where u and $\{f_i\}_{i=1}^N$ are related via

$$f_i = u(x_i) + \sqrt{\varepsilon}\eta_i.$$

Here we assume that the noise $\eta_i \sim \mathcal{N}(0, \sigma_i^2)$. In our Bayesian approach, we build an ε -dependent prior $\tilde{\mu}_\varepsilon$ so that samples drawn from the prior are approximately binary. Formally the prior measure is given by

$$\tilde{\mu}_\varepsilon(du) \propto \exp\left(-\int_{-1}^1 \frac{1}{2}|u'(x)|^2 + \frac{1}{\varepsilon^2}V(u(x))dx\right) du.$$

As a result of Bayes' theorem, the posterior measure $\tilde{\nu}_\varepsilon$ satisfies that

$$\frac{d\tilde{\nu}_\varepsilon}{d\tilde{\mu}_\varepsilon}(u) \propto \exp\left(-\frac{1}{2\varepsilon} \sum_{i=1}^N \lambda_i(u(x_i) - f_i)^2\right)$$

where $\lambda_i = 1/(2\sigma_i^2)$, $i = 1, \dots, N$. Moreover, the MAP estimator of $\tilde{\nu}_\varepsilon$ is the minimiser of Onsager-Machlup functional

$$F_\varepsilon(u) := \int_{-1}^1 \frac{\varepsilon}{2}|u'(x)|^2 + \frac{1}{\varepsilon}V(u(x))dx + \frac{1}{2} \sum_{i=1}^N \lambda_i(u(x_i) - f_i)^2$$

over the functional space of $H_{\pm}^1(-1, 1)$. We understand the asymptotic behaviour of the posterior measure from two perspectives. Firstly we identify the limit of the MAP estimator by identifying the Γ -limit of F_{ε} . We emphasise that this Γ -limit does not follow directly from the stability property of Γ -convergence under continuous perturbation, since the data-fidelity term of the functional F_{ε} involves pointwise evaluations which are not continuous functionals of L^1 -functions. Secondly, we study the concentration phenomenon of the posterior measure $\tilde{\nu}_{\varepsilon}$. Intuitively, the measure should concentrate on a manifold which consists of the minimisers of the Γ -limit of F_{ε} . We justify this rigorously in a simple situation where only two measurements are taken in the inverse problem. In this case the attracted manifold where the posterior is concentrated can be characterised explicitly.

1.5.3 Chapter 5 – Gaussian Approximations for Transition Paths

A Gaussian approximation framework was introduced in the analysis of general finite dimensional probability measures in Chapter 3. We extend the use of such framework to the infinite dimensional transition path problem. More specifically, we are concerned with the “most likely transition paths” in the overdamped Langevin dynamical model. The Freidlin-Wentzell theory identifies the most likely paths in the zero temperature limit via the large deviation principle; the Onsager-Muchlup theory defines the optimal paths at finite temperature in terms of MAP estimator of the underlying path-space probability measure. Unfortunately, the Onsager-Muchlup approach can produce non-physical paths and these paths do not agree with the Freidlin-Wentzell paths when the transition time grows up to infinity as the temperature decreases to zero.

We give an alternative description of typical transition paths in the small temperature regime. The key idea is to seek the best Gaussian approximation, with respect to the Kullback-Leibler divergence, of the non-Gaussian distribution of the diffusion process. We interpret the mean of this Gaussian approximation as the most likely paths and the covariance operator as a means to capture the typical fluctuations around this most likely path. The Gaussian measure used in the approximation is given as the distribution of some time-inhomogeneous Ornstein-Uhlenbeck process, which is parametrised by two parameters, with one specifying the mean and the other controlling the covariance. We formulate the measure approximation as a variational problem with respect to the two parameters and we prove the existence of minimisers for the variational problem. Then the low temperature limit of the Gaussian approximation is studied via the Γ -convergence of the associated variational problem. The limiting functional consists of two parts: The first part only depends on the mean and coincides with the Γ -limit of the Freidlin-Wentzell rate functional. The second part depends on both the mean and the covariance operator and is minimised if the dynamics of approximation is given by an Ornstein-Uhlenbeck process found by linearisation of the

Langevin dynamics around the Freidlin-Wentzell minimiser.

1.5.4 Chapter 6 – A Bayesian Level Set Method for Geometric Inverse Problems

In this chapter we present a Bayesian level set approach to geometric inverse problems. The inverse problem considered here is to find a physical parameter κ from observations $y \in \mathbf{R}^d$ where

$$y = G(\kappa) + \eta,$$

where η is the noise and G is the forward map. Moreover, we assume that κ is known a priori to be piece-wise constants with the form $\kappa(x) = \sum_{i=1}^n \kappa_i \mathbf{I}_{D_i}(x)$ where the constants $\{\kappa_i\}_{i=1}^n$ are assumed to be known and the domains $\{D_i\}_{i=1}^n$ are the only unknowns of interest. Our Bayesian level set method infers the unknown domains in three steps. In the primary step, similar to classical level set methods, each unknown domain D_i is represented by a continuous level set function u via

$$D_i = \{x \in D \mid c_{i-1} \leq u(x) < c_i\}.$$

The function κ is then linked with the level set function u by the level set map, defined by

$$(Fu)(x) \rightarrow \kappa(x) = \sum_{i=1}^n \kappa_i \mathbf{I}_{D_i}(x).$$

Then we seek the posterior probability distribution on the level set function u given y , given a prior probability distribution on u and an independent probabilistic specification of the noise η . Finally the push-forward of the posterior measure of u through the level set map gives rise to a measure of κ from which we can statistically estimate the unknown geometries.

This probabilistic formulation gives a number of advances over classical level set method. Firstly with an appropriate choice of prior the set of discontinuities of the level set map has null probability; this leads to a well-posed inverse problem in which the posterior distribution is Lipschitz with respect to the observed data, from which one can not only estimate interface locations, but also quantify uncertainties in them. Secondly it leads to computationally expedient algorithms in which the level set itself is updated implicitly via the MCMC methodology applied to the level set function — no explicit velocity field is required for the level set interface. We demonstrate the effectiveness of the Bayesian level set method with computational results of two applications: a subsurface flow problem and an inverse source problem.

Chapter 2

Mathematical Preliminaries

2.1 Gaussian Measures

This section collects some basic results about Gaussian measures in infinite dimensional spaces. We start by defining a Gaussian measure on separable Banach spaces. Let X be a Banach space. We say a measure μ is a Borel measure on X if μ is a measure defined on the σ -algebra $\mathcal{B}(X)$ of Borel sets in X . Let $f : X \mapsto Y$ be a map between Banach spaces X and Y . We say f is a Borel measurable function if $f^{-1}(A) \in \mathcal{B}(X)$ for any Borel set A in the σ -algebra $\mathcal{B}(Y)$. We denote by $f^*\mu$ the push-forward of the measure μ under the map f . Note that $f^*\mu$ is a Borel measure in Y if f is a Borel measurable function.

Definition 2.1.1. *A Gaussian measure μ on a separable Banach space X is a Borel measure such that $\ell^*\mu$ is a Gaussian probability measure on \mathbf{R} for every continuous linear functional $\ell : X \mapsto \mathbf{R}$. The measure μ is called centred if $\ell^*\mu$ has mean zero for every $\ell \in X^*$.*

The following fundamental theorem characterises the exponential tail of Gaussian measures and will be useful in controlling integrals against Gaussian measures.

Theorem 2.1.2 (Fernique). *Let μ be a Gaussian measure on a separable Banach space X . Then there exists $a > 0$ such that $\int_X \exp(a\|x\|^2)\mu(dx) < \infty$.*

As an important consequence of the Fernique theorem, a Gaussian measure has finite moments of arbitrary order. In particular, it allows to define the covariance operator as follows. The covariance $C_\mu : X^* \mapsto X$ of a Gaussian measure μ is a bounded linear operator such that

$$C_\mu \ell = \int_X x \ell(x) \mu(dx)$$

for any $\ell \in X^*$.

Now we turn to the discussion of Gaussian measures on separable Hilbert spaces. In the Hilbert space setting, the covariance of a Gaussian measure is more than just a bounded operator, but is also trace class, as shown in the following proposition [110, Proposition 3.15]. Recall that a bounded linear operator A defined on a separable Hilbert space \mathcal{H} with orthonormal bases $\{e_k\}_{k \in \mathbb{N}}$ is trace class if $\text{Tr}(A) := \sum_k (Ae_k, e_k) < \infty$.

Proposition 2.1.3. *A Gaussian measure μ on a separable Hilbert space \mathcal{H} has covariance operator $C_\mu : \mathcal{H} \mapsto \mathcal{H}$ which is trace class and satisfies*

$$\int_{\mathcal{H}} \|x\|^2 \mu(dx) = \text{Tr}(C_\mu).$$

Conversely, for every positive trace-class symmetric operator on \mathcal{H} , there exists a Gaussian measure μ on \mathcal{H} such that $C_\mu = K$.

Given $h \in X$, define the map T_h on X by $T_h(x) = x + h$. The following Cameron-Martin theorem [44, 110] characterises precisely when a centred Gaussian measure μ (in a Hilbert space) is equivalent or singular to its shift $T_h^* \mu$.

Theorem 2.1.4 (Cameron-Martin). *Let $\mu = N(0, C_\mu)$ be a centred Gaussian measure on a Hilbert space \mathcal{H} . Then the measure $T_h^* \mu$ is absolutely continuous with respect to μ if and only if $h \in \mathcal{H}_\mu := \{x \in \mathcal{H} : \|C_\mu^{-\frac{1}{2}} x\| < \infty\}$. Moreover, in the latter case, its Radon-Nikodym derivative is given by*

$$\frac{dT_h^* \mu}{d\mu}(x) = \exp \left(\langle C_\mu^{-\frac{1}{2}} h, C_\mu^{-\frac{1}{2}} x \rangle - \|C_\mu^{-\frac{1}{2}} h\|^2 \right).$$

The space \mathcal{H}_μ in the above theorem is usually referred to as the Cameron-Martin space (or reproducing kernel Hilbert space) associated to the measure μ . It can be shown (by e.g. [21, Proposition 2.4.6]) that the Cameron-Martin space \mathcal{H}_μ is compactly embedded into its underlying Hilbert space \mathcal{H} . Moreover, the Cameron-Martin space \mathcal{H}_μ is a “small” set in \mathcal{H} since as shown in [110, Proposition 3.42] it holds that $\mu(\mathcal{H}_\mu) = 0$. This demonstrates the fact that measures on infinite dimensional spaces are more likely to be mutually singular.

Example 2.1.5 (Brownian Bridge). *Let B_t be a one dimensional Brownian bridge process on $(0, 1)$, that is a Brownian motion W_t subject to the condition that $W(1) = 0$. More precisely,*

$$B_t = (W_t | W_1 = 0), t \in [0, 1]$$

with $B_0 = 0$. The law of $\{B_t : t \in [0, 1]\}$ can be viewed as the centred Gaussian measure $\mu_0 = N(0, C_\mu)$ on the Hilbert space $\mathcal{H} = L^2(0, 1)$ where the covariance operator $C = (-\frac{d^2}{dx^2})^{-1}$ with Dirichlet boundary condition. Let $\mu = N(m, C)$ be another Gaussian

measure with $m \in \mathcal{H}$. It follows from Theorem 2.1.4 that μ and μ_0 are equivalent if and only if $m \in \mathcal{H}_\mu = H_0^1(0, 1)$. Moreover, the Radon-Nikodym derivative is given by

$$\frac{d\mu}{d\mu_0}(x) = \exp(\langle m, x \rangle_{H^1} - |m|_{H^1}^2).$$

2.2 Probability Metrics

In this section, we introduce some probability metrics on the space of probability measures and then discuss some of their important properties and relationships. These metrics quantify the distance between probability measures and will be useful in discussing the well-posedness of Bayesian inverse problems as well as the approximation of probability measures.

Suppose that we are given two probability measures μ and μ' on a measurable space (X, \mathcal{F}) . Then the total variation distance is given as follows.

Definition 2.2.1. *The total variation distance between probability measures μ and μ' is*

$$d_{TV}(\mu, \mu') = \sup_{A \in \mathcal{F}} |\mu(A) - \mu'(A)|.$$

The total variation distance has an equivalent formulation

$$d_{TV}(\mu, \mu') = \frac{1}{2} \int_X \left| \frac{d\mu}{d\nu} - \frac{d\mu'}{d\nu} \right| d\nu,$$

where ν is a common reference measure with respect to which both μ and μ' are absolutely continuous.

Definition 2.2.2. *The Hellinger distance between probability measures μ and μ' is*

$$d_{Hell}(\mu, \mu') = \left(\frac{1}{2} \int_X \left(\sqrt{\frac{d\mu}{d\nu}} - \sqrt{\frac{d\mu'}{d\nu}} \right)^2 d\nu \right)^{\frac{1}{2}}.$$

It follows from the definitions that $0 \leq d(\mu, \mu') \leq 1$ where d stands for d_{TV} or d_{Hell} . Moreover, the total variation distance and the Hellinger distance are related through the following inequality. The proof can be found in [61, Lemma 6.12].

Lemma 2.2.3. *Given two probability measures μ and μ' . Then*

$$\frac{1}{\sqrt{2}} d_{TV}(\mu, \mu') \leq d_{Hell}(\mu, \mu') \leq \frac{1}{\sqrt{2}} d_{TV}(\mu, \mu')^{\frac{1}{2}}.$$

Finally, we introduce the Kullback-Leibler divergence as another measure of the closeness of probability distributions. In Chapter 3 and Chapter 5, the KL-divergence will be used as the cost functional in the variational problems arising from Gaussian approximations for probability measures.

Definition 2.2.4. *The Kullback-Leibler divergence between probability measures μ' and μ , with μ' absolutely continuous with respect to μ , is*

$$D_{KL}(\mu' || \mu) = \mathbb{E}^\mu \left[\frac{d\mu'}{d\mu} \log \left(\frac{d\mu'}{d\mu} \right) d\mu \right] = \int_X \frac{d\mu'}{d\mu} \log \left(\frac{d\mu'}{d\mu} \right) d\mu.$$

If μ' is not absolutely continuous with respect to μ , then the divergence is set to be $+\infty$. It is important to note that the KL-divergence is not a metric since both symmetry and triangle inequality are violated. Nevertheless, the divergence possesses several advantages over previously defined probability metrics in practice. First, in many cases the logarithmic structure of the KL-divergence enables us to calculate the divergence explicitly (see Chapter 5). Second, as shown in the following lemma (cf. [61]), the KL-divergence provides an upper bound for both the total variation distance and the Hellinger distance.

Lemma 2.2.5. *Let μ and μ' are two equivalent probability measures. Then it holds that*

$$d_{TV}(\mu, \mu') \leq \sqrt{D_{KL}(\mu || \mu')}, \quad d_{Hell}(\mu, \mu') \leq \sqrt{\frac{1}{2} D_{KL}(\mu || \mu')}. \quad (2.1)$$

The first inequality of above is also known as Pinsker's inequality [60].

2.3 Onsager-Machlup Functional and MAP Estimator

In this section we recall the definitions of the Onsager-Machlup functional and the *maximum a posteriori* estimator of a probability measure on an infinite dimensional space. Let μ be a probability measure defined on a Banach space X . For $z \in X$, denote by $B_\delta(z)$ the open ball of radius δ centred at z .

Definition 2.3.1. *If there exists a functional I , defined on $E \subset X$, such that for $z_1, z_2 \in E$,*

$$\lim_{\delta \downarrow 0} \frac{\mu(B_\delta(z_2))}{\mu(B_\delta(z_1))} = I(z_1) - I(z_2),$$

then I is called the Onsager-Machlup functional of μ .

Definition 2.3.2. *For a fixed $\delta > 0$, let $z_\delta = \arg \max_{z \in X} \mu(B_\delta(z))$. Then a point $z \in X$*

is called the MAP estimator of the measure μ if

$$\lim_{\delta \downarrow 0} \frac{\mu(B_\delta(z))}{\mu(B_\delta(z_\delta))} = 1.$$

The MAP estimator is not unique in general and it is interpreted as a “most likely” point of a probability measure in the sense of maximising the small ball probabilities. In many applications, the measure of interest, μ , has a density with respect a reference measure μ_0 :

$$\frac{d\mu}{d\mu_0}(u) \propto \exp(-\Psi(u))du. \quad (2.2)$$

Here μ_0 is a Gaussian measure $N(m, C)$ on X with the Cameron-Martin space $(E, \langle \cdot, \cdot \rangle_E)$. In this case, the existence of the MAP estimator is guaranteed under some assumptions [63] on the potential function Ψ .

Assumption 2.3.3. *The function $\Psi : X \mapsto \mathbf{R}$ satisfies the following properties.*

(i) *For every $\varepsilon > 0$, there is an $M \in \mathbf{R}$ such that for all $u \in X$,*

$$\Psi(u) \geq M - \varepsilon \|u\|_X^2.$$

(ii) *Ψ is locally bounded from above, i.e. for every $r > 0$, there exists $K = K(r) > 0$ such that, for all $u \in X$ with $\|u\|_X < r$, we have $\Psi(u) \leq K$.*

(iii) *Ψ is locally Lipschitz continuous, i.e. for every $r > 0$, there exists $L = L(r) > 0$ such that, for all $u_1, u_2 \in X$ with $\max(\|u_1\|_X, \|u_2\|_X) < r$, we have*

$$|\Psi(u_1) - \Psi(u_2)| \leq L \|u_1 - u_2\|_X.$$

Theorem 2.3.4. *Let μ be the measure defined by (2.2) with Ψ satisfying Assumption 2.3.3. Then*

(i) *The Onsager-Machlup functional of μ is given by*

$$I(u) := \begin{cases} \Psi(u) + \frac{1}{2} \|u - m\|_E^2 & \text{if } u - m \in E, \text{ and} \\ +\infty & \text{otherwise .} \end{cases}$$

(ii) *The MAP estimator of μ is given by the minimiser of I defined as above.*

Proof. See Theorem 3.2 and Theorem 3.5 of [63]. □

2.4 Γ -convergence

The notion of Γ -convergence, since its first introduction by De Giorgi [107], has become a predominant notion in calculus of variations and partial differential equations for the study of the convergence of functionals. Typical applications of the Γ -convergence include the gradient theory of phase transition [25], homogenisation theory [27] and the free continuity problems arising in image analysis [11]. For a detailed treatment of the general theory of Γ -convergence, we refer the reader to the books of Braides [25] and Dal Maso [164]. In this thesis, Γ -convergence will be used as a natural framework to characterise the asymptotic convergence of probability measures.

We first recall the following definition of Γ -convergence.

Definition 2.4.1. *Let X be a metric space and $E_\varepsilon : X \rightarrow \mathbf{R}$ a family of functionals indexed by $\varepsilon > 0$. Then E_ε Γ -converges to $E : X \rightarrow \mathbf{R}$ as $\varepsilon \rightarrow 0$ if the following conditions hold:*

- (i) (liminf inequality) *for every $u \in X$, and for every sequence $u_\varepsilon \in X$ such that $u_\varepsilon \rightarrow u$, it holds that $E(u) \leq \liminf_{\varepsilon \downarrow 0} E_\varepsilon(u_\varepsilon)$;*
- (ii) (limsup inequality) *for every $u \in X$ there exists a recovery sequence $\{u_\varepsilon\}$ such that $u_\varepsilon \rightarrow u$ and $E(u) \geq \limsup_{\varepsilon \downarrow 0} E_\varepsilon(u_\varepsilon)$.*

We say a sequence of functionals $\{E_\varepsilon\}$ is compact if $\limsup_{\varepsilon \downarrow 0} E_\varepsilon(u_\varepsilon) < \infty$ implies that there exists a subsequence $\{u_{\varepsilon_j}\}$ such that $u_{\varepsilon_j} \rightarrow u \in X$.

Proposition 2.4.2. [164, Proposition 6.8] *If $E_\varepsilon \xrightarrow{\Gamma} E$ in X , then E is lower-semi continuous on X .*

As a consequence of Proposition 2.4.2, the Γ -limit has a minimiser if the minimising sequence admits a compact subsequence. Moreover, the following proposition shows that the Γ -convergence is stable with respect to continuous perturbation (cf. [164, Proposition 6.21]).

Proposition 2.4.3. *If $E_\varepsilon \xrightarrow{\Gamma} E$, then for any continuous functional G , $G + E_\varepsilon \xrightarrow{\Gamma} G + E$.*

The following fundamental theorem of Γ -convergence states that

$$\Gamma - \text{convergence} + \text{compactness} \implies \text{convergence of minima}.$$

This property makes Γ -convergence particularly appealing in characterising the limiting behaviour of minimisers of variational problems. We remark that the compactness property in Definition 2.4.1 is also called *equi-coerciveness* in the literature; see e.g. [25, 164].

Theorem 2.4.4 (Convergence of minima). *Suppose that $\limsup_{\varepsilon \downarrow 0} E_\varepsilon(u_\varepsilon) < \infty$. Let u_ε be a minimiser of E_ε . If $\{E_\varepsilon\}$ is compact and Γ -converges to E , then there exists a subsequence u_{ε_j} such that $u_{\varepsilon_j} \rightarrow u$ where u is a minimiser of E .*

Proof. We refer the proof of this proposition to [164, Chapter 7] and [26, Chapter 2]. \square

To give a concrete example of Γ -convergence, we consider identifying the Γ -limit of the Ginzburg-Landau energy functional. To that end, let V be a double-well potential taking $\{\pm 1\}$ as its minimisers. For example $V(u) := \frac{1}{4}(1 - u^2)^2$. We define the Ginzburg-Landau energy functional E_ε associated to V by

$$E_\varepsilon(u) := \int_{-1}^1 \frac{\varepsilon}{2} |u'(x)|^2 + \frac{1}{\varepsilon} V(u(x)) dx \quad (2.3)$$

with $u \in H^1(-1, 1)$ and $\varepsilon > 0$. The Ginzburg-Landau model arises in the gradient theory of phase transitions in material sciences; see the celebrated work by Van der Waals [66] and Cahn-Hilliard [39]. In a material, for example a fluid, a configuration of the system may be described by a function u which approximately takes constant values in different regions (representing different phases), like ± 1 in the above model, and smoothly transits from one phase to the other. The parameter ε describes the width of the transition layer. In Van der Waals's theory, the stable configurations of fluid are characterised by the function u_ε which minimises the energy functional E_ε . Physically in the equilibrium the interface separating two phases should minimise the surface area; this is justified via the asymptotic analysis of E_ε in the limit $\varepsilon \rightarrow 0$. The follow lemma proves the Γ -convergence of E_ε .

Lemma 2.4.5. *Let E_ε be a functional defined in (2.3). Then E_ε Γ -converges to the perimeter functional*

$$E(u) := \begin{cases} c_0 \# S(u) & \text{if } u \in BV((-1, 1); \{-1, 1\}) \\ +\infty & \text{otherwise in } L^1(-1, 1) \end{cases}$$

with respect to L^1 -topology. Here $S(u)$ denotes the jump set of a binary function u over $(-1, 1)$ and the constant c_0 represents the minimal cost for each jump that is given by

$$c_0 := \int_{-1}^1 \sqrt{2V(u)} du.$$

The proof of Lemma 2.4.5 is firstly due to Modica-Mortola [171] (see also [170]). Since then Modica-Mortola's result had been generalised to the vector valued cases in [214] and [96]. Later Baldo [12] extended their results further allowing both vector density function and multiple (more than two) phases.

Chapter 3

Gaussian Approximations for Probability Measures on \mathbb{R}^d

3.1 Introduction

In this paper, we study the “best” approximation of a general finite dimensional probability measure, which could be non-Gaussian, from a set of simple probability measures, such as a single Gaussian measure or a Gaussian mixture family. We define “best” to mean the measure within the simple class which minimizes the Kullback-Leibler divergence between itself and the target measure. This type of approximation is central to many ideas, especially including the so-called “variational inference” [227], that are widely used in machine learning [19]. Yet such approximation has not been the subject of any substantial systematic underpinning theory. The purpose of this paper is to develop such a theory in the concrete finite dimensional setting in two ways: (i) by establishing the existence of best approximations; (ii) by studying their asymptotic properties in a measure concentration limit of interest. The abstract theory is then applied to study frequentist consistency [65] of Bayesian inverse problems.

3.1.1 Background and Overview

The idea of approximation for probability measures with respect to Kullback-Leibler divergence has been applied in a number of areas; see for example [138, 159, 161, 205]. Despite the wide usage of Kullback-Leibler approximation, systematic theoretical study has only been initiated recently. In [187], the measure approximation problem is studied from the calculus of variations point of view, and the existence of minimisers is established therein. The companion paper [190] proposed numerical algorithms for implementing Kullback-Leibler minimisation in practice. In [159], Gaussian approximation is used as

a new approach for identifying the most likely path between equilibrium states in molecular dynamics; furthermore, the asymptotic behaviour of the Gaussian approximation in the small temperature limit is analysed via Γ -convergence. Here our interest is to develop the ideas in [159] in the context of a general class of measure approximation problems in finite dimensions.

To be concrete we consider approximation of a family of probability measures $\{\mu_\varepsilon\}_{\varepsilon>0}$ on \mathbf{R}^d with Lebesgue density of the form

$$\mu_\varepsilon(dx) = \frac{1}{Z_{\mu,\varepsilon}} \exp\left(-\frac{1}{\varepsilon}V_1^\varepsilon(x) - V_2(x)\right) dx. \quad (3.1)$$

Here $Z_{\mu,\varepsilon}$ is the normalisation constant. A typical example of a measure μ_ε with this form is a posterior measure in Bayesian inverse problems. For instance, consider the inverse problem of identifying x from a sequence of noisy observations $\{y_j\}_{j \in \mathbb{N}}$ where

$$y_j = G(x) + \eta_j,$$

and where the η_j denote describe the random noise terms. This may model a statistical measurement with an increasing number of observations or with vanishing noise. In the Bayesian approach to this inverse problem, if we take a prior with density proportional to $\exp(-V_2(x))$, then the posterior measure is given by (3.1) with the function $\varepsilon^{-1}V_1^\varepsilon$, up to an additive constant, coinciding with the negative log-likelihood. The parameter ε is associated with the number of observations or the noise level of the statistical experiment.

Our study of Gaussian approximation to the measures μ_ε in (3.1) is partially motivated by the famous Bernstein-von Mises (BvM) theorem [65] in asymptotic statistics. Roughly speaking, the BvM theorem states that under mild conditions on the prior, the posterior distribution of a Bayesian procedure converges to a Gaussian distribution centred at any consistent estimator (for instance the maximum likelihood estimator) in the limit of large data (or, relatedly, small noise [33]). The BvM theorem is of great importance in Bayesian statistics for at least two reasons. First, it gives a quantitative description of how the posterior contracts to the underlying truth. Second, it implies that the Bayesian credible sets are asymptotically equivalent to frequentist confidence intervals and hence the estimation of the latter can be realised by making use of the computational power of Markov Chain Monte Carlo algorithms. We interpret the BvM phenomenon in the abstract theoretical framework of best Gaussian approximations with respect to a Kullback-Leibler measure of divergence.

3.1.2 Main Contributions

The main contributions of this chapter are twofold:

- We use the calculus of variations to give a framework to the problem of finding the best Gaussian (mixture) approximation of a given measure, with respect to a Kullback-Leibler divergence;
- We study the resulting calculus of variations problem in the small noise (or large data) limits, thereby making new links to, and ways to think about, the classical Bernstein-von Mises theory of asymptotic normality.

We describe these contributions in more detail. First we introduce a theoretical framework of calculus of variations to analyse the measure approximation problem. Given a measure μ_ε defined by (3.1), we find a measure ν_ε from a set of simple measures, Gaussians or mixtures of finitely many Gaussians, which minimises the Kullback-Leibler divergence $D_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$. We characterise the limiting behaviour of the best approximation ν_ε as well as the limiting behaviour of the Kullback-Leibler divergence as $\varepsilon \downarrow 0$ using the framework of Γ -convergence. In particular, if μ_ε is a multimodal distribution and ν_ε is the best approximation from within the class of Gaussian mixtures, then the limit of the minimised KL-divergence $D_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$ can be characterised explicitly as the sum of two contributions: a local term which consists of a weighted sum of the KL-divergences between the Gaussian approximations, as well as the Gaussian measure whose covariance is determined by the Hessian of V_2 at its minimisers; and a global term which measures how well the weights approximate the mass distribution between the modes; see Theorem 3.4.2.

We then adopt the abstract measure approximation theory to understanding the posterior consistency of finite dimensional Bayesian inverse problems. In particular, we give an alternative (and more analytical) proof of the Bernstein-von Mises theorem, see Theorem 3.5.4 and Corollary 3.5.5. We highlight the fact that our BvM result improves classical BvM results for parametric statistical models in two aspects. Firstly, the convergence of posterior in the total variation distance is improved to convergence in the KL-divergence, under certain regularity assumptions on the forward map. Secondly, our BvM result allows the posterior distribution to be multimodal, in which case the posterior approaches a mixture of Gaussian distributions rather than a single Gaussian distribution in the limit of infinite data. These improvements come at a cost, and we need to make stronger assumptions than those made in classical BvM theory.

3.1.3 Structure

The rest of the chapter is organised as follows. In Section 3.2.1 and Section 3.2.2 we spell out the assumptions made and the notation used. In Section 3.3 and Section 3.4 we study the problem of approximation of the measure μ_ε by, respectively, a single Gaussian measure and a Gaussian mixture. In particular, the small ε asymptotics of the Gaussians (or Gaussian mixtures) are captured by using the framework of Γ -convergence. In Section 3.5, the theory which we have developed is applied to understand the posterior consistency for Bayesian inverse problems, and connections to the BvM theory. Finally, we finish in Section 5.5 with several conclusion remarks.

3.2 Set-Up

3.2.1 Assumptions

Throughout the chapter, we make the following assumptions on the potential functions V_1^ε and V_2 which define the target measure of interest.

Assumption 3.2.1.

(A-1) For any $\varepsilon > 0$, V_1^ε and V_2 are non-negative functions in the space $C^4(\mathbf{R}^d)$ and $C^2(\mathbf{R}^d)$ respectively. Moreover, there exist constants $\varepsilon_0 > 0$ and $M_V > 0$ such that, when $\varepsilon < \varepsilon_0$,

$$|\partial_x^\alpha V_1^\varepsilon(x)| \vee \left| \partial_x^\beta V_2(x) \right| \leq M_V e^{|x|^2}$$

for any $|\alpha| \leq 4, |\beta| \leq 2$ and all $x \in \mathbf{R}^d$.

(A-2) There exists $n > 0$ such that when $\varepsilon \ll 1$, the set of minimisers of V_1^ε is $\mathcal{E}^\varepsilon = \{x_\varepsilon^1, x_\varepsilon^2, \dots, x_\varepsilon^n\}$ and $V_1^\varepsilon(x_\varepsilon^i) = 0, i = 1, \dots, n$.

(A-3) There exists V_1 such that $V_1^\varepsilon \rightarrow V_1$ pointwise. The limit V_1 has n distinct global minimisers which are given by

$$\mathcal{E} = \{x^1, x^2, \dots, x^n\}.$$

For each $i = 1, \dots, n$ the Hessian $D^2V_1(x^i)$ is positive definite.

(A-4) The convergence $x_\varepsilon^i \rightarrow x^i$ holds.

(A-5) There exist constants $c_0, c_1 > 0$ and $\varepsilon_0 > 0$ such that when $\varepsilon < \varepsilon_0$,

$$V_1^\varepsilon(x) \geq -c_0 + c_1|x|^2, x \in \mathbf{R}^d.$$

Remark 3.2.2. Conditions (A-2)-(A-4) mean that for sufficiently small $\varepsilon > 0$, the function V_1^ε behaves like a quadratic function in the neighbourhood of the minimisers x_ε^i and of x^i . Consequently, the measure μ_ε is asymptotically normal in the local neighbourhood of x_ε^i . In particular, in conjunction with Condition (A-5) this implies that there exists $\delta > 0$ and $C_\delta > 0$ such that $\forall 0 \leq \eta < \delta$,

$$\text{dist}(x, \mathcal{E}) \geq \eta \implies \liminf_{\varepsilon \downarrow 0} V_1^\varepsilon(x) \geq C_\delta |\eta|^2. \quad (3.2)$$

Remark 3.2.3. The local boundedness of V_1^ε in $C^4(\mathbf{R}^d)$ (Assumption (A-1)) together with the pointwise convergence of V_1^ε to V_1 (Assumption (A-3)) implies the much stronger locally uniform convergence of derivatives up to order 3. Furthermore, (A-4) then implies that $V_1^\varepsilon(x_\varepsilon^i) \rightarrow V_1(x^i)$ and $D^2 V_1^\varepsilon(x_\varepsilon^i) \rightarrow D^2 V_1(x^i)$.

3.2.2 Notation

Throughout the chapter, C and \tilde{C} will be generic constants which are independent of the quantities of interest, and may change from line to line. Let $\mathcal{S}_\geq(\mathbf{R}, d)$ and $\mathcal{S}_>(\mathbf{R}, d)$ be the set of all $d \times d$ real matrices which are positive semi-definite or positive definite, respectively. Denote by $N(m, \Sigma)$ a Gaussian measure with mean m and covariance matrix Σ . We use $|\mathbf{A}|$ to denote the Frobenius norm of the $d \times d$ matrix \mathbf{A} , namely $|\mathbf{A}| = \sqrt{\text{Tr}(\mathbf{A}^T \mathbf{A})}$. We denote by $\lambda_{\min}(\mathbf{A})$ the smallest eigenvalue of \mathbf{A} . We let $B(x, r)$ denote a ball in \mathbf{R}^d with centre x and radius r . Given a random variable η , we use \mathbb{E}^η and \mathbb{P}^η when computing the expectation and the probability under the law of η respectively.

3.3 Approximation by Single Gaussian Measures

Let \mathcal{A} be the set of Gaussian measures on \mathbf{R}^d , given by

$$\mathcal{A} = \{N(m, \Sigma) : m \in \mathbf{R}^d, \Sigma \in \mathcal{S}_\geq(\mathbf{R}, d)\}.$$

The set \mathcal{A} is closed with respect to weak convergence of probability measures. Consider the variational problem

$$\inf_{\nu \in \mathcal{A}} D_{\text{KL}}(\nu || \mu_\varepsilon). \quad (3.3)$$

Given $\nu = N(m, \Sigma) \in \mathcal{A}$, the Kullback-Leibler divergence $D_{\text{KL}}(\nu||\mu_\varepsilon)$ can be calculated explicitly as

$$\begin{aligned} D_{\text{KL}}(\nu||\mu_\varepsilon) &= \mathbb{E}^\nu \log \left(\frac{d\nu}{d\mu_\varepsilon} \right) \\ &= \frac{1}{\varepsilon} \mathbb{E}^\nu V_1^\varepsilon(x) + \mathbb{E}^\nu V_2(x) - \log \sqrt{(2\pi)^d \det \Sigma} - \frac{d}{2} + \log Z_{\mu, \varepsilon}. \end{aligned} \quad (3.4)$$

If Σ is non-invertible then $D_{\text{KL}}(\nu||\mu_\varepsilon) = +\infty$. The term $-\frac{d}{2}$ comes from the expectation $\mathbb{E}^\nu \frac{1}{2}(x-m)^T \Sigma (x-m)$ and is independent of Σ . The term $-\log \sqrt{(2\pi)^d \det \Sigma}$ prevents the measure ν from being too close to a Dirac measure. The following theorem shows that the problem (3.3) has a solution.

Theorem 3.3.1. *Consider the measure μ_ε given by (3.1). For any $\varepsilon > 0$, there exists at least one probability measure $\bar{\nu}_\varepsilon \in \mathcal{A}$ solving the problem (3.3).*

Proof. We first show that the infimum of (3.3) is finite. In fact, consider $\nu^* = N(0, \frac{1}{4}\mathbf{I}_d)$. Under the Assumption 5.2.1 (A-1) we have that

$$\mathbb{E}^{\nu^*} V_1^\varepsilon(x) \vee \mathbb{E}^{\nu^*} V_2(x) \leq \frac{M_V}{\sqrt{(2\pi \times \frac{1}{4})^d}} \int_{\mathbf{R}^d} e^{-\frac{4}{2}|x|^2 + |x|^2} dx < \infty.$$

Note that the integral in the last expression is finite due to $-\frac{4}{2} + 1 < 0$. Hence we know from (3.4) that $\inf_{\nu \in \mathcal{A}} D_{\text{KL}}(\nu||\mu_\varepsilon) < \infty$. Then the existence of minimisers follows from the fact that the Kullback-Leibler divergence has compact sub-level sets and the closedness of \mathcal{A} with respect to weak convergence of probability measures; see e.g. [187, Corollary 2.2]. \square

We aim to understand the asymptotic behaviour of the minimisers $\bar{\nu}_\varepsilon$ of the problem (3.3) as $\varepsilon \downarrow 0$. Due to the factor $\frac{1}{\varepsilon}$ in front of V_1^ε in the definition of μ_ε , (3.1), we expect the typical size of fluctuations around the minimisers to be of order $\sqrt{\varepsilon}$ and we reflect that in our choice of scaling. More precisely, for $m \in \mathbf{R}^d$, $\Sigma \in \mathcal{S}_{\geq}(\mathbf{R}, d)$ we define $\nu_\varepsilon = N(m, \varepsilon \Sigma)$ and set

$$F_\varepsilon(m, \Sigma) := D_{\text{KL}}(\nu_\varepsilon||\mu_\varepsilon). \quad (3.5)$$

Understanding the asymptotic behaviour of minimisers $\bar{\nu}_\varepsilon$ in the small ε limit may be achieved by understanding Γ -convergence of the functional F_ε .

To that end, we define weights

$$\beta^i = (\det D^2 V_1(x^i))^{-\frac{1}{2}} \cdot e^{-V_2(x^i)}, \quad i = 1, \dots, n,$$

and the counting probability measure on $\{1, \dots, n\}$ given by

$$\beta := \frac{1}{\sum_{j=1}^n \beta^j} (\beta^1, \dots, \beta^n).$$

Intuitively, as $\varepsilon \downarrow 0$, we expect the measure μ_ε to concentrate on the set $\{x^i\}$ with weights on each x^i given by β ; this intuition is reflected in the asymptotic behaviour of the normalisation constant $Z_{\mu, \varepsilon}$, as we now show. By definition,

$$Z_{\mu, \varepsilon} = \int_{\mathbf{R}^d} \exp \left(-\frac{1}{\varepsilon} V_1^\varepsilon(x) - V_2(x) \right) dx.$$

The following lemma follows from the Laplace approximation for integrals (see e.g. [134]) and Assumption 5.2.1 (A-4).

Lemma 3.3.2. *Let V_1^ε and V_2 satisfy Assumption 5.2.1. Then as $\varepsilon \downarrow 0$,*

$$Z_{\mu, \varepsilon} = \sqrt{(2\pi\varepsilon)^d} \cdot \left(\sum_{i=1}^n \beta^i \right) \cdot (1 + o(1)). \quad (3.6)$$

Recall from (3.5) that $F_\varepsilon(m, \Sigma) = D_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$ with the specific scaling $\nu_\varepsilon = N(m, \varepsilon \Sigma)$. In view of the expression (3.4) for the Kullback-Leibler divergence, it follows from Lemma (3.3.2) that

$$F_\varepsilon(m, \Sigma) = \frac{1}{\varepsilon} \mathbb{E}^{\nu_\varepsilon} V_1^\varepsilon(x) + \mathbb{E}^{\nu_\varepsilon} V_2(x) - \frac{d}{2} - \frac{1}{2} \log(\det \Sigma) + \log \left(\sum_{i=1}^n \beta^i \right) + o(1). \quad (3.7)$$

Armed with this analysis of the normalisation constant we may now prove the following theorem which identifies the Γ -limit of F_ε . To this end we define

$$F_0(m, \Sigma) := V_2(m) + \frac{1}{2} \text{Tr} \left(D^2 V_1(m) \cdot \Sigma \right) - \frac{d}{2} - \frac{1}{2} \log \det \Sigma + \log \left(\sum_{i=1}^n \beta^i \right).$$

Theorem 3.3.3. *The Γ -limit of F_ε is*

$$F(m, \Sigma) := \begin{cases} F_0(m, \Sigma) & \text{if } m \in \mathcal{E} \text{ and } \Sigma \in \mathcal{S}_{>}(\mathbf{R}, d), \\ \infty & \text{otherwise.} \end{cases} \quad (3.8)$$

The following corollary follows directly from the Γ -convergence of F_ε .

Corollary 3.3.4. *Let $\{(m_\varepsilon, \Sigma_\varepsilon)\}$ be a family of minimisers of $\{F_\varepsilon\}$. Then there exists a subsequence $\{\varepsilon_k\}$ such that $(m_{\varepsilon_k}, \Sigma_{\varepsilon_k}) \rightarrow (m, \Sigma)$ and $F_{\varepsilon_k}(m_{\varepsilon_k}, \Sigma_{\varepsilon_k}) \rightarrow F(m, \Sigma)$. Moreover, (m, Σ) is a minimiser of F .*

Before we give the proof of Theorem 3.3.3, let us first discuss the limit functional F as well as its minimisation. We assume that $m = x^{i_0}$ for some $i_0 \in \{1, \dots, n\}$ and rewrite the definition of $F_0(x^{i_0}, \Sigma)$, by adding and subtracting

$$\log(\beta^{i_0}) = -V_2(x^{i_0}) - \frac{1}{2} \log((\det D^2 V_1(x^{i_0})))$$

and cancelling the terms involving $V_2(x^{i_0})$ as

$$\begin{aligned} F_0(x^{i_0}, \Sigma) &= \frac{1}{2} \text{Tr}(D^2 V_1(x^{i_0}) \cdot \Sigma) - \frac{d}{2} - \frac{1}{2} \log \det(D^2 V_1(x^{i_0}) \cdot \Sigma) \\ &\quad + \log \left(\sum_{i=1}^n \beta^i \right) - \log(\beta^{i_0}). \end{aligned} \quad (3.9)$$

Now it is interesting to see that the first line of (3.9) gives the Kullback-Leibler divergence $D_{\text{KL}}(N(x^{i_0}, \Sigma) \parallel N(x^{i_0}, (D^2 V_1(x^{i_0}))^{-1}))$. The second line of (3.9) is equal to the Kullback-Leibler divergence $D_{\text{KL}}(\mathbf{e}^{i_0} \parallel \beta)$, for $\mathbf{e}^{i_0} := (0, \dots, 1, \dots, 0)$. In conclusion,

$$F_0(x^i, \Sigma) = D_{\text{KL}}(N(x^i, \Sigma) \parallel N(x^i, (D^2 V_1(x^i))^{-1})) + D_{\text{KL}}(\mathbf{e}^i \parallel \beta), \quad (3.10)$$

in other words, in the limit $\varepsilon \downarrow 0$, the Kullback-Leibler divergence between the best Gaussian measure ν_ε and the measure μ_ε consists of two parts: the first part is the relative entropy between the Gaussian measure with rescaled covariance Σ and the Gaussian measure with covariance determined by $(D^2 V_1(x^i))^{-1}$; the second part is the relative entropy between the Dirac mass supported at x^i and a weighted sum of Dirac masses, with weights β , at the $\{x^j\}_{j=1}^n$. Clearly, to minimise $F_0(m, \Sigma)$, on the one hand, we need to choose $m = x^i$ and $\Sigma = (D^2 V_1(x^i))^{-1}$ for some $i \in 1, \dots, n$; for this choice the first term on the right side of (3.9) vanishes. In order to minimise the second term we need to choose the minimum x^i with maximal weight β^i . In particular, the following corollary holds.

Corollary 3.3.5. *The minimum of F_0 is zero when $n = 1$, but it is strictly positive when $n > 1$.*

Corollary 3.3.5 reflects the fact that, in the limit $\varepsilon \downarrow 0$, a single Gaussian measure is not the best choice for approximating a non-Gaussian measure with multiple modes; this motivates our study of Gaussian mixtures in Section 3.4.

The proofs of Theorem 3.3.3 and Corollary 3.3.4 are provided after establishing a sequence of lemmas. The following lemma shows that the sequence of functionals $\{F_\varepsilon\}$ is compact (recall Definition 2.4.1). It is well known that the Kullback-Leibler divergence (with respect to a fixed reference μ) has compact sub-level sets with respect to weak convergence of probability measures. Here we prove a stronger statement, which is specific to

the family of reference measures μ_ε , namely a uniform bound from above and below for the rescaled covariances, i.e. we prove a bound from above and below for Σ_ε if we control $F_\varepsilon(m_\varepsilon, \Sigma_\varepsilon)$.

Lemma 3.3.6. *Let $\{(m_\varepsilon, \Sigma_\varepsilon)\} \subset \mathbf{R}^d \times \mathcal{S}_\geq(\mathbf{R}, d)$ be such that $\limsup_{\varepsilon \downarrow 0} F_\varepsilon(m_\varepsilon, \Sigma_\varepsilon) < \infty$. Then*

$$0 < \liminf_{\varepsilon \downarrow 0} \lambda_{\min}(\Sigma_\varepsilon) < \limsup_{\varepsilon \downarrow 0} \text{Tr}(\Sigma_\varepsilon) < \infty \quad (3.11)$$

and $\text{dist}(m_\varepsilon, \mathcal{E}) \downarrow 0$ as $\varepsilon \downarrow 0$. In particular, there exist common subsequences $\{m_k\}_{k \in \mathbb{N}}$ of $\{m_\varepsilon\}$, $\{\Sigma_k\}_{k \in \mathbb{N}}$ of $\{\Sigma_\varepsilon\}$ such that $m_k \rightarrow x_{i_0}$ with $1 \leq i_0 \leq n$ and $\Sigma_k \rightarrow \Sigma \in \mathcal{S}_>(\mathbf{R}, d)$.

Proof. Let $M := \limsup_{\varepsilon \downarrow 0} F_\varepsilon(m_\varepsilon, \Sigma_\varepsilon) < \infty$. Since m_ε and Σ_ε are defined in finite dimensional spaces, we only need to show that both sequences are uniformly bounded. The proof consists of the following steps.

Step 1. We first prove the following rough bound for $\text{Tr}(\Sigma_\varepsilon)$: there exists positive constants C_1, C_2 such that when $\varepsilon \ll 1$,

$$C_1 \leq \text{Tr}(\Sigma_\varepsilon) \leq \frac{C_2}{\varepsilon}. \quad (3.12)$$

In fact, from the formula (3.7) and the assumption that V_1^ε and V_2 are non-negative, we can get that when $\varepsilon \ll 1$

$$\log(\det \Sigma_\varepsilon) \geq 2(C_V - M - 1) \quad (3.13)$$

where the constant

$$C_V := -\frac{d}{2} + \log \left(\sum_{i=1}^n \beta^i \right).$$

Then the lower bound of (3.12) follows from (3.13) and the arithmetic-geometric mean inequality

$$\det \mathbf{A} \leq \left(\frac{1}{d} \text{Tr}(\mathbf{A}) \right)^d \quad (3.14)$$

which holds for any positive definite \mathbf{A} . In addition, using the condition (A-5) for the

potential V_1^ε , we obtain from (3.7) that when $\varepsilon \ll 1$,

$$\begin{aligned}
M &\geq F_\varepsilon(m_\varepsilon, \mathbf{A}_\varepsilon) \\
&\geq \mathbb{E}^{\nu_\varepsilon} V_2(x) + \frac{c_1}{\varepsilon} \mathbb{E}^{\nu_\varepsilon} |x|^2 - \frac{c_0}{\varepsilon} - \frac{1}{2} \log(\det \mathbf{\Sigma}_\varepsilon) + C_V - 1 \\
&= \mathbb{E}^{\nu_\varepsilon} V_2(x) + c_1 \text{Tr}(\mathbf{\Sigma}_\varepsilon) + \frac{c_1 |m_\varepsilon|^2}{\varepsilon} - \frac{c_0}{\varepsilon} - \frac{1}{2} \log(\det \mathbf{\Sigma}_\varepsilon) + C_V - 1 \\
&\geq c_1 \text{Tr}(\mathbf{\Sigma}_\varepsilon) - \frac{c_0}{\varepsilon} - \frac{1}{2} \log \left(\left(\frac{1}{d} \text{Tr}(\mathbf{\Sigma}_\varepsilon) \right)^d \right) + C_V - 1 \\
&= c_1 \text{Tr}(\mathbf{\Sigma}_\varepsilon) - \frac{c_0}{\varepsilon} - \frac{d}{2} \log(\text{Tr}(\mathbf{\Sigma}_\varepsilon)) + \frac{d \log d}{2} + C_V - 1,
\end{aligned} \tag{3.15}$$

where we have used the inequality (3.14) and the assumption that V_2 is non-negative. Dropping the non-negative terms on the right hand side we rewrite this expression as an estimate on $\text{Tr}(\mathbf{\Sigma}_\varepsilon)$:

$$c_1 \text{Tr}(\mathbf{\Sigma}_\varepsilon) - \frac{d}{2} \log(\text{Tr}(\mathbf{\Sigma}_\varepsilon)) \leq M + \frac{c_0}{\varepsilon} + 1,$$

and conclude that there exists $C_2 > 0$ such that $\text{Tr}(\mathbf{\Sigma}_\varepsilon) \leq C_2/\varepsilon$ by observing that for $x \gg 1$ we have $c_1 x - \frac{d}{2} \log x \geq \frac{c_1}{2} x$.

Step 2. In this step we show that for $\varepsilon \ll 1$ the mass of ν_ε concentrates near the minimisers. More precisely, we claim that there exist constants $R_1, R_2 > 0$, such that for every $\varepsilon \ll 1$ there exists an index $i_0 \in \{1, 2, \dots, n\}$ such that

$$\nu_\varepsilon \left(B \left(x_{i_0}, \sqrt{\varepsilon(R_1 + R_2 \log(\det \mathbf{\Sigma}_\varepsilon))} \right) \right) \geq \frac{1}{2n}. \tag{3.16}$$

On the one hand, from the expression (3.7) and the assumption that

$$\limsup_{\varepsilon \downarrow 0} F_\varepsilon(m_\varepsilon, \mathbf{\Sigma}_\varepsilon) \leq M$$

we know that there exist $C_3, C_4 > 0$ such that when $\varepsilon \ll 1$

$$\mathbb{E}^{\nu_\varepsilon} V_1^\varepsilon(x) \leq \varepsilon (C_3 + C_4 \log(\det \mathbf{\Sigma}_\varepsilon)). \tag{3.17}$$

On the other hand, it follows from (3.2) that for $\eta \ll 1$

$$\begin{aligned}
\mathbb{E}^{\nu_\varepsilon} V_1^\varepsilon(x) &\geq \mathbb{E}^{\nu_\varepsilon} \left[V_1^\varepsilon(x) \mathbf{I}_{(\cup_{i=1}^n B(x_i, \eta))^c}(x) \right] \\
&\geq C_\delta \eta^2 \nu_\varepsilon(\cup_{i=1}^n B(x_i, \eta))^c,
\end{aligned} \tag{3.18}$$

which combined with (3.17) leads to

$$\nu_\varepsilon(\cup_{i=1}^n B(x_i, \eta))^c \leq \varepsilon \frac{(C_3 + C_4 \log(\det \Sigma_\varepsilon))}{C_\delta \eta^2}. \quad (3.19)$$

Now we choose $\eta = \eta_\varepsilon := \sqrt{2\varepsilon(C_3 + C_4 \log(\det \Sigma_\varepsilon))/C_\delta}$ (by the rough bound (3.12) this η_ε tends to zero as $\varepsilon \rightarrow 0$, which permits to apply (3.2)). This implies (3.16) with $R_1 = \frac{2C_3}{C_\delta}$ and $R_2 = \frac{2C_4}{C_\delta}$, by passing to the complement and observing that

$$\sup_{i \in \{1, \dots, n\}} \nu_\varepsilon(B(x_i, \eta_\varepsilon)) \geq \frac{1}{n} \nu_\varepsilon(\cup_{i \in \{1, \dots, n\}} B(x_i, \eta_\varepsilon)).$$

Step 3. We prove the bound (3.11). As in the previous step we set

$$\eta_\varepsilon = \sqrt{\varepsilon(R_1 + R_2 \log(\det \Sigma_\varepsilon))}.$$

It follows from (3.16) that

$$\begin{aligned} \frac{1}{2n} &\leq \nu_\varepsilon(B(x_{i_0}, \eta_\varepsilon)) \\ &= \frac{1}{\sqrt{(2\pi\varepsilon)^d \det \Sigma_\varepsilon}} \int_{B(x_{i_0}, \eta_\varepsilon)} \exp\left(-\frac{1}{2\varepsilon} \langle x - m_\varepsilon, \Sigma_\varepsilon^{-1}(x - m_\varepsilon) \rangle\right) dx \\ &\leq \frac{1}{\sqrt{(2\pi\varepsilon)^d \det \Sigma_\varepsilon}} |B(x_{i_0}, \eta_\varepsilon)| \\ &\leq C \frac{1}{\sqrt{\varepsilon^d \det \Sigma_\varepsilon}} \eta_\varepsilon^d \leq C \sqrt{\frac{(R_1 + R_2 \log(\det \Sigma_\varepsilon))^d}{\det \Sigma_\varepsilon}}. \end{aligned} \quad (3.20)$$

This implies that $\limsup_{\varepsilon \downarrow 0} \det \Sigma_\varepsilon < C$ for some $C > 0$. In order to get a lower bound on individual eigenvalues $\Lambda_\varepsilon^{(i)}$ of Σ_ε , we rewrite the same integral in a slightly different way. We use the change of coordinates $y = \frac{\mathbf{P}_\varepsilon^T(x - m_\varepsilon)}{\sqrt{\varepsilon}}$, where \mathbf{P}_ε is orthogonal and diagonalises Σ_ε and observe that under this transformation $B(x^i, \eta_\varepsilon)$ is mapped into $B(\frac{x^i - m}{\sqrt{\varepsilon}}, \frac{\eta_\varepsilon}{\varepsilon}) \subseteq \{y: |y_j - \frac{(x^i - m)}{\sqrt{\varepsilon}}| \leq \frac{\eta_\varepsilon}{\varepsilon} \text{ for } j = 1, \dots, n\}$. This yields

$$\begin{aligned} \frac{1}{2n} &\leq \frac{1}{\sqrt{(2\pi)^d \det \Sigma_\varepsilon}} \int_{\{|y_j - \frac{(x^i - m)}{\sqrt{\varepsilon}}| \leq \frac{\eta_\varepsilon}{\varepsilon}\}} \exp\left(-\frac{1}{2} \langle y_i, (\Lambda_\varepsilon^{(i)})^{-1} y_i \rangle\right) dy \\ &\leq \frac{1}{\sqrt{(2\pi)^d \det \Sigma_\varepsilon}} \left(\frac{2\eta_\varepsilon}{\sqrt{\varepsilon}}\right)^{d-1} \int_{\mathbf{R}} \exp\left(-\frac{|y_i|^2}{2\Lambda_\varepsilon^{(i)}}\right) dy_i \\ &= \sqrt{\frac{\Lambda_\varepsilon^{(i)}}{(2\pi)^d \det \Sigma_\varepsilon}} (R_1 + R_2 \log(\det \Sigma_\varepsilon))^{\frac{d-1}{2}} \end{aligned} \quad (3.21)$$

for any $i \in \{1, 2, \dots, d\}$. Together with the uniform boundedness of $\det \Sigma_\varepsilon$ this implies that $\Lambda_\varepsilon^{(i)} > C'$ for some $C' > 0$. Finally,

$$\text{Tr}(\Sigma_\varepsilon) = \sum_{i=1}^d \Lambda_\varepsilon^{(i)} = \sum_{i=1}^d \frac{\det(\Sigma_\varepsilon)}{\prod_{j=1, j \neq i}^d \Lambda_\varepsilon^{(j)}} \leq \frac{dC}{(C')^{d-1}} < \infty. \quad (3.22)$$

This proves (3.11).

Step 4. We show that $\text{dist}(m_\varepsilon, \mathcal{E}) \downarrow 0$ as $\varepsilon \downarrow 0$. On the one hand, by the upper bound on the variance in (3.11) and standard Gaussian concentration, we see that there exists a constant $c > 0$, such that for $\varepsilon \ll 1$ we have $\nu_\varepsilon(B(m_\varepsilon, \sqrt{\varepsilon}c)) \geq \frac{3}{4}$. On the other hand, we had already seen in (3.19) that for $\eta = \eta_\varepsilon$ we have

$$\nu_\varepsilon(\cup_{i=1}^n B(x_i, \eta_\varepsilon))^c \leq \frac{1}{2},$$

and hence $B(m_\varepsilon, \sqrt{\varepsilon}c)$ must intersect at least one of the $B(x_i, \eta_\varepsilon)$. This yields for this particular index i

$$|x_i - m_\varepsilon| \leq \eta_\varepsilon + \sqrt{\varepsilon}c,$$

and establishes the claim. □

Lemma 3.3.7. *Let $\{(m_\varepsilon, \Sigma_\varepsilon)\}$ be a sequence such that $\limsup_{\varepsilon \downarrow 0} |m_\varepsilon| =: C_1 < \infty$ and*

$$0 < c_2 := \liminf_{\varepsilon \downarrow 0} \lambda_{\min}(\Sigma_\varepsilon) < \limsup_{\varepsilon \downarrow 0} \text{Tr}(\Sigma_\varepsilon) =: C_2 < \infty.$$

Then as $\varepsilon \downarrow 0$,

$$\begin{aligned} F_\varepsilon(m_\varepsilon, \Sigma_\varepsilon) &= \frac{V_1^\varepsilon(m_\varepsilon)}{\varepsilon} + V_2(m_\varepsilon) + \frac{1}{2} \text{Tr}(D^2 V_1^\varepsilon(m_\varepsilon) \cdot \Sigma_\varepsilon) - \frac{1}{2} \log \left((2\pi\varepsilon)^d \det \Sigma_\varepsilon \right) \\ &\quad - \frac{d}{2} + \log Z_{\mu, \varepsilon} + r_\varepsilon \end{aligned} \quad (3.23)$$

where $|r_\varepsilon| \leq C\varepsilon$ with $C = C(C_1, c_2, C_2, M_V)$ (Recall that M_V is the constant defined in Assumption 5.2.1 (A-I)).

Proof. The lemma follows directly from the expression (3.4) and Taylor expansion. Indeed, we first expand V_2 near m_ε up to the first order and then take expectation to get

$$\mathbb{E}^{\nu_\varepsilon} V_2(x) = V_2(m_\varepsilon) + \mathbb{E}^{\nu_\varepsilon} R_\varepsilon(x)$$

with the residual

$$R_\varepsilon(x) = \sum_{|\alpha|=2} \frac{(x - m_\varepsilon)^\alpha}{\alpha!} \int_0^1 \partial^\alpha V_2(\xi x + (1 - \xi)m_\varepsilon) (1 - \xi)^2 d\xi.$$

Thanks to the condition (A-1), one can obtain the bound

$$\begin{aligned} \mathbb{E}^{\nu_\varepsilon} R_\varepsilon(x) &\leq \sum_{|\alpha|=2} \frac{1}{\alpha!} \max_{\xi \in [0,1]} \left\{ \mathbb{E}^{\nu_\varepsilon} \left[|x - m_\varepsilon|^2 \partial^\alpha V_2(\xi x + (1 - \xi)m_\varepsilon) \right] \right\} \\ &\leq \frac{M_V}{\sqrt{(2\pi\varepsilon)^d \det \Sigma_\varepsilon}} \max_{\xi \in [0,1]} \left\{ \int_{\mathbf{R}^d} |x|^2 e^{(|x|+|m_\varepsilon|)^2} \cdot e^{-\frac{1}{2\varepsilon} x^T \Sigma_\varepsilon^{-1} x} dx \right\} \\ &\leq \frac{M_V}{\sqrt{(2\pi\varepsilon)^d \det \Sigma_\varepsilon}} e^{2|m_\varepsilon|^2} \int_{\mathbf{R}^d} |x|^2 e^{-\frac{1}{2\varepsilon} x^T (\Sigma_\varepsilon^{-1} - 4\varepsilon \cdot \mathbf{I}_d) x} dx \\ &= \frac{M_V \varepsilon}{\sqrt{\det \Sigma_\varepsilon}} e^{2|m_\varepsilon|^2} \cdot \det(\Sigma_\varepsilon^{-1} - 4\varepsilon \cdot \mathbf{I}_d)^{-1} \\ &\leq C\varepsilon, \end{aligned} \tag{3.24}$$

when $\varepsilon \ll 1$. Note that in the last inequality we have used the assumption that all eigenvalues of Σ_ε are bounded from above which ensures that for $\varepsilon \ll 1$ the matrix $\Sigma_\varepsilon^{-1} - 4\varepsilon \cdot \mathbf{I}_d$ is positive definite. Hence

$$\mathbb{E}^{\nu_\varepsilon} V_2(x) = V_2(m_\varepsilon) + r_{1,\varepsilon}$$

with $r_{1,\varepsilon} \leq C\varepsilon$ as $\varepsilon \downarrow 0$. Similarly, one can take the fourth order Taylor expansion for V_1^ε near m_ε and then take expectation to obtain that

$$\mathbb{E}^{\nu_\varepsilon} V_1^\varepsilon(x) = \frac{V_1^\varepsilon(m_\varepsilon)}{\varepsilon} + \frac{1}{2} \text{Tr} (D^2 V_1^\varepsilon(m_\varepsilon) \cdot \Sigma_\varepsilon) + r_{2,\varepsilon}$$

with $r_{2,\varepsilon} \leq C\varepsilon$. Then (3.23) follows directly by inserting the above equations into the expression (3.4). \square

The following corollary is a direct consequence of Lemma 3.3.2, Lemma 3.3.6 and Lemma 3.3.7, providing an asymptotic formula for $F_\varepsilon(m_\varepsilon, \Sigma_\varepsilon)$ as $\varepsilon \downarrow 0$.

Corollary 3.3.8. *Let $\{(m_\varepsilon, \Sigma_\varepsilon)\} \subset \mathbf{R}^d \times \mathcal{S}_\geq(\mathbf{R}, d)$ be such that $\limsup_{\varepsilon \downarrow 0} F_\varepsilon(m_\varepsilon, \Sigma_\varepsilon) < \infty$. Then for $\varepsilon \ll 1$*

$$\begin{aligned} F_\varepsilon(m_\varepsilon, \Sigma_\varepsilon) &= \frac{V_1^\varepsilon(m_\varepsilon)}{\varepsilon} + V_2(m_\varepsilon) + \frac{1}{2} \text{Tr}(D^2 V(m_\varepsilon) \cdot \Sigma_\varepsilon) - \frac{1}{2} \log(\det \Sigma_\varepsilon) \\ &\quad - \frac{d}{2} + \sum_{i=1}^n \beta^i + o(1). \end{aligned} \tag{3.25}$$

Remark 3.3.9. We do not have a bound on the convergence rate for the residual expression (3.25), because Lemma 3.3.2 does not provide a convergence rate on the $Z_{\mu,\varepsilon}$. This is because we do not impose any rate of convergence for the convergence of the x_ε^i to x^i . The bound $|r_\varepsilon| \leq C\varepsilon$ in Lemma 3.3.7 will be used to prove the rate of convergence for the posterior measures that arise from Bayesian inverse problems; see Theorem 3.5.4 in Section 3.5, and its proof.

Proof of Theorem 3.3.3. We first prove the liminf inequality. Let $(m_\varepsilon, \Sigma_\varepsilon)$ be such that $m_\varepsilon \rightarrow m$ and $\Sigma_\varepsilon \rightarrow \Sigma$. We want to show that $F(m, \Sigma) \leq \liminf_{\varepsilon \downarrow 0} F_\varepsilon(m_\varepsilon, \Sigma_\varepsilon)$. We may assume that $\liminf_{\varepsilon \downarrow 0} F_\varepsilon(m_\varepsilon, \Sigma_\varepsilon) < \infty$ since otherwise there is nothing to prove. By Lemma 3.3.6 this implies that $m \in \mathcal{E}$ and that Σ is positive definite. Then the liminf inequality follows from (3.25) and the fact that $V_1^\varepsilon \geq 0$.

Next we show the limsup inequality is true. Given $m \in \mathcal{E}$, $\Sigma \in \mathcal{S}_{>}(\mathbf{R}, d)$, we want to find a recovery sequence (m_k, Σ_k) such that $(m_k, \Sigma_k) \rightarrow (m, \Sigma)$ and $\limsup_k F_{\varepsilon_k}(m_k, \Sigma_k) \leq F(m, \Sigma)$. In fact, we set $\Sigma_k = \Sigma$. Moreover, by Assumption 5.2.1 (A-4), we can choose $\{m_k\}$ to be one of the zeros of $V_1^{\varepsilon_k}$ so that $V_1^{\varepsilon_k}(m_k) = 0$ and $m_k \rightarrow m \in \mathcal{E}$. This implies that $V_2(m_k) \rightarrow V_2(m)$. Then the limsup inequality follows from (3.25). \square

Proof of Corollary 3.3.4. First we show $\limsup_{\varepsilon \downarrow 0} F_\varepsilon(m_\varepsilon, \Sigma_\varepsilon) < \infty$. In fact, let $\tilde{m}_\varepsilon = x_\varepsilon^1$ and $\tilde{\Sigma}_\varepsilon = D^2 V_1^\varepsilon(x_\varepsilon^1)$. It follows from (3.25) that $\limsup_{\varepsilon \downarrow 0} F_\varepsilon(\tilde{m}_\varepsilon, \tilde{\Sigma}_\varepsilon) < \infty$. According to Theorem 2.4.4, the convergence of minima and minimisers is a direct consequence of Lemma 3.3.6 and Theorem 3.3.3. \square

3.4 Approximation by Gaussian Mixtures

In the previous section we demonstrated the approximation of the target measure (3.1) by a Gaussian. Corollary 3.3.5 shows that, when the measure has only one mode, this approximation is perfect in the limit $\varepsilon \rightarrow 0$: the limit KL-divergence tends to zero since both entropies in (3.10) tend to zero. However when multiple modes exist, and persist in the small ε limit, the single Gaussian is inadequate because the relative entropy term $D_{\text{KL}}(e^\dagger || \beta)$ can not be small even though the relative entropy between Gaussians tends to zero. In this section we consider the approximation of the target measure μ_ε by Gaussian mixtures in order to overcome this issue. We show that in the case of n minimisers of V_1 , the approximation with a mixture of n Gaussians is again perfect as $\varepsilon \rightarrow 0$. The Gaussian mixture model is widely used in the pattern recognition and machine learning community; see the relevant discussion in [19, Chapter 9].

Let Δ^n be the standard n -simplex, i.e.,

$$\Delta^n = \left\{ \alpha = (\alpha^1, \alpha^2, \dots, \alpha^n) \in \mathbf{R}^n : \alpha^i \geq 0 \text{ and } \sum_{i=1}^n \alpha^i = 1 \right\}.$$

For $\xi \in (0, 1)$, we define $\Delta_\xi^n = \{ \alpha = (\alpha^1, \alpha^2, \dots, \alpha^n) \in \mathbf{R}^n : \alpha^i \geq \xi \}$.

Recall that \mathcal{A} is the set of Gaussian measures and define the set of Gaussian mixtures

$$\mathcal{M}_n = \left\{ \nu = \sum_{i=1}^n \alpha^i \nu^i : \nu^i \in \mathcal{A}, \alpha = (\alpha^1, \alpha^2, \dots, \alpha^n) \in \Delta^n \right\}. \quad (3.26)$$

Also, for a fixed $\xi = (\xi_1, \xi_2) \in (0, 1) \times (0, \infty)$ we define the set

$$\begin{aligned} \mathcal{M}_n^\xi = \left\{ \nu = \sum_{i=1}^n \alpha^i \nu^i : \nu^i = N(m^i, \Sigma^i) \in \mathcal{A} \text{ with } \min_{i \neq j} |m^i - m^j| \geq \xi_2, \right. \\ \left. \alpha = (\alpha^1, \alpha^2, \dots, \alpha^n) \in \Delta_{\xi_1}^n \right\}. \end{aligned} \quad (3.27)$$

The set \mathcal{M}_n is the set of all convex combinations of n Gaussians taken from \mathcal{A} and the set \mathcal{M}_n^ξ can be seen as an “effective” version of \mathcal{M}_n , in which each Gaussian component plays an active role, and no two Gaussians share a common centre.

Consider the problem of minimising $D_{\text{KL}}(\nu || \mu_\varepsilon)$ within \mathcal{M}_n or \mathcal{M}_n^ξ . Since the sets \mathcal{M}_n and \mathcal{M}_n^ξ are both closed with respect to weak convergence, we have the following existence result whose proof is similar to Theorem 3.3.1 and is omitted.

Theorem 3.4.1. *Consider the measure μ_ε given by (3.1) with fixed $\varepsilon > 0$, and the problem of minimising the functional*

$$\nu \mapsto D_{\text{KL}}(\nu || \mu_\varepsilon) \quad (3.28)$$

from the set \mathcal{M}_n , or from the set \mathcal{M}_n^ξ with some fixed $\xi = (\xi_1, \xi_2) \in (0, 1) \times (0, \infty)$. In both cases, there exists at least one minimiser to the functional (3.28).

Now we continue to investigate the asymptotic behaviour of the Kullback-Leibler approximations based on Gaussian mixtures. To that end, we again parametrise a measure ν in the set \mathcal{M}_n or \mathcal{M}_n^ξ by the weights $\alpha = (\alpha^1, \alpha^2, \dots, \alpha^n)$ as well as the n means as well as the n covariances matrices. Similar to the previous section we need to chose the right scaling in our Gaussian mixtures to reflect the typical size of fluctuations of μ_ε . Thus

for $\mathbf{m} = (m^1, m^2, \dots, m^n)$ and $\Sigma = (\Sigma^1, \Sigma^2, \dots, \Sigma^n)$, we set

$$\nu_\varepsilon = \sum_{i=1}^n \alpha^i N(m^i, \varepsilon \Sigma^i). \quad (3.29)$$

We can view $D_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$ as a functional of $(\alpha, \mathbf{m}, \Sigma)$ and study the Γ -convergence of the resulting functional. For that purpose, we need to restrict our attention to finding the best Gaussian mixtures within \mathcal{M}_n^ξ for some $\xi \in (0, 1) \times (0, \infty)$. The reasons are the following. First, we require individual Gaussian measures ν^i to be active (i.e. $\alpha^i > \xi_1 > 0$) because $D_{\text{KL}}(\nu_\varepsilon, \mu_\varepsilon)$, as a family of functionals of $(\alpha, \mathbf{m}, \Sigma)$ indexed by ε , is not compact if we allow some of the α^i to vanish. In fact, if $\alpha_\varepsilon^i = 0$ for some $i \in 1, 2, \dots, n$, then $D_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$ is independent of m_ε^i and Σ_ε^i . In particular, if $|m_\varepsilon^i| \wedge |\Sigma_\varepsilon^i| \rightarrow \infty$ while $|m_\varepsilon^j| \vee |\Sigma_\varepsilon^j| < \infty$ for all the j 's such that $j \neq i$, then it still holds that $\limsup_{\varepsilon \downarrow 0} D_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon) < \infty$. Second, it makes more sense to assume that the individual Gaussian means stay apart from each other (i.e. $\min_{i \neq j} |m^i - m^j| \geq \xi_2 > 0$) since we primarily want to locate different modes of the target measure. Moreover, it seems impossible to identify a sensible Γ -limit without such an assumption; see Remark 3.4.7.

Recall that the measure ν has the form (3.29). Let $\xi = (\xi_1, \xi_2) \in (0, 1) \times (0, \infty)$ be fixed. In view of these considerations it is useful to define

$$S_\xi = \{(\alpha, \mathbf{m}) \in \Delta_{\xi_1}^n \times \mathbf{R}^{nd} : \min_{i \neq j} |m^i - m^j| \geq \xi_2\}.$$

We define the functional

$$G_\varepsilon(\alpha, \mathbf{m}, \Sigma) := \begin{cases} D_{\text{KL}}(\nu || \mu_\varepsilon) & \text{if } (\alpha, \mathbf{m}) \in S_\xi, \\ +\infty & \text{otherwise.} \end{cases} \quad (3.30)$$

By the definition of the Kullback-Leibler divergence, if $(\alpha, \mathbf{m}) \in S_\xi$, then

$$G_\varepsilon(\alpha, \mathbf{m}, \Sigma) = \int \rho(x) \log \rho(x) dx + \frac{1}{\varepsilon} \mathbb{E}^\nu V_1^\varepsilon(x) + \mathbb{E}^\nu V_2(x) + \log Z_{\mu, \varepsilon} \quad (3.31)$$

where ρ is the probability density function (p.d.f) of ν .

Recall the Γ -limit F defined in (3.8). Then we have the following Γ -convergence result.

Theorem 3.4.2. *The Γ -limit of G_ε is*

$$G(\alpha, \mathbf{m}, \Sigma) := \begin{cases} \sum_{i=1}^n \alpha^i D_{KL}(N(m^i, \Sigma^i) \parallel N(m^i, (D^2 V_1(m^i))^{-1})) \\ \quad + D_{KL}(\alpha \parallel \beta) & \text{if } (\alpha, \mathbf{m}) \in S_\xi \text{ and } m^i \in \mathcal{E} \\ +\infty & \text{otherwise.} \end{cases} \quad (3.32)$$

Remark 3.4.3. *The right hand side of G consists of two parts: the first part is a weighted relative entropy which measures the discrepancy between two Gaussians, and the second part is the relative entropy between sums of Dirac masses at $\{x^j\}_{j=1}^n$ with weights α and β respectively. This has the same spirit as the entropy splitting used in [166, Lemma 2.4].*

Before we prove Theorem 3.4.2, we consider the minimisation of the limit functional G . First let ξ_1, ξ_2 be such that

$$\xi_1 > 0, \quad 0 < \xi_2 \leq \min_{i \neq j} |x^i - x^j|, \quad (3.33)$$

where $\{x^i\}_{i=1}^n$ are the minimisers of V_1 . To minimise G , without loss of generality, we may choose $m^i = \bar{m}^i := x^i$. Then the weighted relative entropy in the first term in the definition (3.32) of G vanishes if we set $\Sigma^i = \bar{\Sigma}^i := D^2 V_1(x^i)^{-1}$. The relative entropy of the weights also vanishes if we choose the weight $\alpha = \bar{\alpha} := \beta$. To summarise, the minimiser $(\bar{\alpha}, \bar{\mathbf{m}}, \bar{\Sigma})$ of G is given by

$$\bar{m}^i = x^i, \quad \bar{\Sigma}^i = D^2 V_1(x^i)^{-1}, \quad \bar{\alpha}^i = \beta^i, \quad (3.34)$$

and $G(\bar{\alpha}, \bar{\mathbf{m}}, \bar{\Sigma}) = 0$. The following corollary is a direct consequence of the Γ -convergence of G_ε .

Corollary 3.4.4. *Let $\{(\alpha_\varepsilon, \mathbf{m}_\varepsilon, \Sigma_\varepsilon)\}$ be a family of minimisers of $\{G_\varepsilon\}$. Then there exists a subsequence $\{\varepsilon_k\}$ such that $(\alpha_{\varepsilon_k}, \mathbf{m}_{\varepsilon_k}, \Sigma_{\varepsilon_k}) \rightarrow (\bar{\alpha}, \bar{\mathbf{m}}, \bar{\Sigma})$ and that $G_{\varepsilon_k}(\alpha_{\varepsilon_k}, \mathbf{m}_{\varepsilon_k}, \Sigma_{\varepsilon_k}) \rightarrow G(\bar{\alpha}, \bar{\mathbf{m}}, \bar{\Sigma})$. Moreover, $(\bar{\alpha}, \bar{\mathbf{m}}, \bar{\Sigma})$ is a minimiser of G and $G(\bar{\alpha}, \bar{\mathbf{m}}, \bar{\Sigma}) = 0$.*

For a non-Gaussian measure μ_ε with multiple modes, i.e., $n > 1$ in the Assumption 5.2.1, we have seen in Corollary 3.3.5 that the Kullback-Leibler divergence between μ_ε and the best Gaussian measure selected from \mathcal{A} remains positive as $\varepsilon \downarrow 0$. However, this gap is filled by using Gaussian mixtures, namely, with ν_ε being chosen as the best Gaussian mixture, the Kullback-Leibler divergence $D_{KL}(\nu_\varepsilon \parallel \mu_\varepsilon) \downarrow 0$ as $\varepsilon \downarrow 0$.

Similarly to the proof of Theorem 3.3.3, Theorem 3.4.2 follows directly from Corollary 3.4.8 below, whose proof requires several lemmas. We start by showing the compactness of $\{G_\varepsilon\}$.

Lemma 3.4.5. Let G_ε be defined by (3.30). Fix $\xi = (\xi_1, \xi_2)$ satisfying the condition (3.33). Let $\{(\alpha_\varepsilon, \mathbf{m}_\varepsilon, \Sigma_\varepsilon)\}$ be a sequence in $S_\xi \times S_{\geq}(\mathbf{R}, d)$ such that

$$\limsup_{\varepsilon \downarrow 0} G_\varepsilon(\alpha_\varepsilon, \mathbf{m}_\varepsilon, \Sigma_\varepsilon) < \infty.$$

Then

$$\liminf_{\varepsilon \downarrow 0} \min_i \lambda_{\min}(\Sigma_\varepsilon^i) > 0, \quad \limsup_{\varepsilon \downarrow 0} \max_i \text{Tr}(\Sigma_\varepsilon^i) < \infty \quad (3.35)$$

and $\text{dist}(m_\varepsilon^i, \mathcal{E}) \downarrow 0$ as $\varepsilon \downarrow 0$. In particular, for any i , there exists $j = j(i) \in \{1, 2, \dots, n\}$ and a subsequence $\{m_k^i\}_{k \in \mathbb{N}}$ of $\{m_\varepsilon^i\}$ such that $m_k \rightarrow x_j$ as $k \rightarrow \infty$.

Proof. We write $M = \limsup_{\varepsilon \downarrow 0} G_\varepsilon(\alpha_\varepsilon, \mathbf{m}_\varepsilon, \Sigma_\varepsilon)$ and $\nu_\varepsilon = \sum_{i=1}^n \alpha_\varepsilon^i \nu_\varepsilon^i$ with $\nu_\varepsilon^i = N(m_\varepsilon^i, \varepsilon \Sigma_\varepsilon^i)$. Then we get

$$\begin{aligned} D_{KL}(\nu_\varepsilon || \mu_\varepsilon) &= \sum_{j=1}^n \alpha_\varepsilon^j \mathbb{E}^{\nu_\varepsilon^j} \log \left(\sum_i \alpha_\varepsilon^i \frac{d\nu_\varepsilon^i}{d\mu_\varepsilon} \right) \\ &\geq \sum_{j=1}^n \alpha_\varepsilon^j \mathbb{E}^{\nu_\varepsilon^j} \log \left(\alpha_\varepsilon^j \frac{d\nu_\varepsilon^j}{d\mu_\varepsilon} \right) \\ &= \sum_{j=1}^n \alpha_\varepsilon^j \log(\alpha_\varepsilon^j) + \sum_{j=1}^n \alpha_\varepsilon^j \mathbb{E}^{\nu_\varepsilon^j} \log \left(\frac{d\nu_\varepsilon^j}{d\mu_\varepsilon} \right) \\ &= \sum_{j=1}^n \alpha_\varepsilon^j \log(\alpha_\varepsilon^j) + \sum_{j=1}^n \alpha_\varepsilon^j D_{KL}(\nu_\varepsilon^j || \mu_\varepsilon) \end{aligned}$$

where the inequality follows simply from the monotonicity of the logarithmic function. As each of term $D_{KL}(\nu_\varepsilon^j || \mu_\varepsilon)$ is non-negative, this implies the bound

$$D_{KL}(\nu_\varepsilon^j || \mu_\varepsilon) \leq \frac{1}{\alpha_\varepsilon^j} \left(M - n \min_{\alpha \in [0,1]} \alpha \log \alpha \right).$$

Using the lower bound $\alpha_\varepsilon^j > \xi_1$ which holds by assumption we get a uniform upper bound on $D_{KL}(\nu_\varepsilon^j || \mu_\varepsilon)$ which in turn permits to invoke Lemma 3.3.6. □

Lemma 3.4.6. Let $\{(\alpha_\varepsilon, \mathbf{m}_\varepsilon, \Sigma_\varepsilon)\}$ be a sequence in $S_\xi \times S_{\geq}(\mathbf{R}, d)$ with $\xi = (\xi_1, \xi_2)$ satisfying (3.33) and such that

$$c_1 \leq \liminf_{\varepsilon \downarrow 0} \min_i \lambda_{\min}(\Sigma_\varepsilon^i) < \limsup_{\varepsilon \downarrow 0} \max_i |m_\varepsilon^i| \vee \text{Tr}(\Sigma_\varepsilon^i) \leq C_1 < \infty.$$

Then

$$\begin{aligned}
& G_\varepsilon(\alpha_\varepsilon, \mathbf{m}_\varepsilon, \Sigma_\varepsilon) \\
&= \sum_{i=1}^n \alpha_\varepsilon^i \left(\frac{V_1^\varepsilon(m_\varepsilon^i)}{\varepsilon} + V_2(m_\varepsilon^i) + \frac{1}{2} \text{Tr}(D^2 V_1^\varepsilon(m_\varepsilon^i) \cdot \Sigma_\varepsilon^i) - \frac{1}{2} \log(\det \Sigma_\varepsilon^i) \right) \\
&+ \sum_{i=1}^n \alpha_\varepsilon^i \log \alpha_\varepsilon^i - \frac{d}{2} + \log Z_{\mu, \varepsilon} + r_\varepsilon.
\end{aligned} \tag{3.36}$$

where $r_\varepsilon \leq C\varepsilon$ with $C = C(c_1, C_1, M_V, \xi_2)$.

Proof. By assumption, we know from (3.31) that

$$G_\varepsilon(\alpha_\varepsilon, \mathbf{m}_\varepsilon, \Sigma_\varepsilon) = \int \rho_\varepsilon(x) \log \rho_\varepsilon(x) dx + \frac{1}{\varepsilon} \mathbb{E}^{\nu_\varepsilon} V_1^\varepsilon(x) + \mathbb{E}^{\nu_\varepsilon} V_2(x) + \log Z_{\mu, \varepsilon}$$

where $\rho_\varepsilon = \sum_{i=1}^n \alpha_\varepsilon^i \rho_\varepsilon^i$ is the probability density of the measure ν_ε . First of all, applying the same Taylor expansion arguments used to obtain (3.23), one can deduce that

$$\begin{aligned}
& \frac{1}{\varepsilon} \mathbb{E}^{\nu_\varepsilon} V_1^\varepsilon(x) + \mathbb{E}^{\nu_\varepsilon} V_2(x) \\
&= \sum_{i=1}^n \alpha_\varepsilon^i \left(\frac{V_1^\varepsilon(m_\varepsilon^i)}{\varepsilon} + \frac{1}{2} \text{Tr}(\nabla^2 V_1^\varepsilon(m_\varepsilon^i) \cdot \Sigma_\varepsilon^i) + V_2(m_\varepsilon^i) \right) + r_{1, \varepsilon}
\end{aligned} \tag{3.37}$$

with $r_{1, \varepsilon} \leq C\varepsilon$ and $C = C(C_1, c_1, M_V)$. Next, we claim that the entropy of ρ_ε can be rewritten as

$$\int \rho_\varepsilon(x) \log \rho_\varepsilon(x) dx = \sum_{i=1}^n \alpha_\varepsilon^i \left(\int \rho_\varepsilon^i(x) \log \rho_\varepsilon^i(x) dx + \log \alpha_\varepsilon^i \right) + r_{2, \varepsilon} \tag{3.38}$$

where $r_{2, \varepsilon} \leq e^{-\frac{C}{\varepsilon}}$ when $\varepsilon \ll 1$ with the constant $C = C(C_1, c_2, \xi_2)$. By definition,

$$\int \rho_\varepsilon(x) \log \rho_\varepsilon(x) dx = \sum_{i=1}^n \alpha_\varepsilon^i \int \rho_\varepsilon^i(x) \log \left(\sum_{j=1}^n \alpha_\varepsilon^j \rho_\varepsilon^j(x) \right) dx,$$

so it suffices to show that for each $i \in \{1, \dots, n\}$ we have

$$\int \rho_\varepsilon^i(x) \log \left(\sum_{j=1}^n \alpha_\varepsilon^j \rho_\varepsilon^j(x) \right) dx = \int \rho_\varepsilon^i(x) \log \rho_\varepsilon^i(x) dx + \log \alpha_\varepsilon^i + r_{2, \varepsilon} \tag{3.39}$$

with $r_{2,\varepsilon} \leq e^{-\frac{C}{\varepsilon}}$. Indeed, the monotonicity of the logarithmic function yields

$$\int \rho_\varepsilon^i(x) \log \left(\sum_{j=1}^n \alpha_\varepsilon^j \rho_\varepsilon^j(x) \right) dx \geq \int \rho_\varepsilon^i(x) \log \rho_\varepsilon^i(x) dx + \log \alpha_\varepsilon^i. \quad (3.40)$$

In order to show the matching lower bound we first recall that the means m_ε^i of the ν_ε^i are well separated by assumption, $\min_{j \neq i} |m_\varepsilon^i - m_\varepsilon^j| > \xi_2$. Let $\delta \ll \frac{\xi_2}{2}$ to be fixed below and set $B_\delta^i = B(m_\varepsilon^i, \delta)$. Then we write

$$\begin{aligned} & \int \rho_\varepsilon^i \log \left(\sum_{j=1}^n \alpha_\varepsilon^j \rho_\varepsilon^j \right) \\ &= \int \rho_\varepsilon^i \log (\alpha_\varepsilon^i \rho_\varepsilon^i) + \int_{B_\delta^i} \rho_\varepsilon^i \left(\log \left(\sum_{j=1}^n \alpha_\varepsilon^j \rho_\varepsilon^j \right) - \log (\alpha_\varepsilon^i \rho_\varepsilon^i) \right) \\ & \quad + \int_{(B_\delta^i)^c} \rho_\varepsilon^i \left(\log \left(\sum_{j=1}^n \alpha_\varepsilon^j \rho_\varepsilon^j \right) - \log (\alpha_\varepsilon^i \rho_\varepsilon^i) \right) \\ &=: \left(\int \rho_\varepsilon^i \log \rho_\varepsilon^i + \log \alpha_\varepsilon^i \right) + E_\varepsilon^1 + E_\varepsilon^2. \end{aligned} \quad (3.41)$$

We first show that the error term E_ε^2 is exponentially small. To that end, we first drop the exponential term in the Gaussian density to obtain the crude bound

$$\log \left(\sum_{j=1}^n \alpha_\varepsilon^j \rho_\varepsilon^j \right) \leq \log \left(\sum_{j=1}^n \alpha_\varepsilon^j \frac{1}{\sqrt{(2\pi\varepsilon)^d \det \Sigma_\varepsilon^j}} \right) \leq \frac{d}{2} \log \varepsilon^{-1} + C. \quad (3.42)$$

where in the second inequality we use the fact that $\det \Sigma_\varepsilon^i$ is bounded away from zero, which has been established in (3.35). Moreover, by definition we have

$$-\log (\alpha_\varepsilon^i \rho_\varepsilon^i) \leq \frac{d}{2} \log \varepsilon^{-1} + C + \frac{|x - m_\varepsilon^i|^2}{\varepsilon}. \quad (3.43)$$

Plugging bounds (3.42) and (3.43) in and using Gaussian concentration as well as the lower bound on λ_{\min} established in Lemma 3.4.5

$$E_\varepsilon^2 \leq \int_{(B_\delta^i)^c} \rho_\varepsilon^i(x) \left(\frac{d}{2} \log \varepsilon^{-1} + C + \frac{|x - m_\varepsilon^i|^2}{\varepsilon} \right) dx \leq C (\log \varepsilon^{-1} + \varepsilon^{-1}) e^{-\frac{C\delta}{\varepsilon}} \quad (3.44)$$

when $\varepsilon \ll 1$. Next, we want to bound E_ε^1 . Notice that $m_\varepsilon^j \rightarrow m^j$ for $j = 1, \dots, n$, hence if $x \in B_\delta^i$ and if $\delta < \xi_1$, then $|x - m_\varepsilon^j| > \xi_1 - \delta$ for any $j \neq i$ when $\varepsilon \ll 1$. As a consequence,

$$\int_{B_\delta^i} \sum_{j=1, j \neq i}^n \alpha_\varepsilon^j \rho_\varepsilon^j \leq C \varepsilon^{-\frac{d}{2}} e^{-\frac{C(\xi_1 - \delta)^2}{\varepsilon}}. \quad (3.45)$$

This together with the elementary inequality

$$\log(x + y) = \log(x) + \int_x^{x+y} \frac{1}{t} dt \leq \log x + \frac{y}{x}$$

for any $x, y > 0$ implies

$$\begin{aligned} E_\varepsilon^1 &= \int_{B_\delta^i} \rho_\varepsilon^i \left(\log \left(\alpha_\varepsilon^i \rho_\varepsilon^i + \sum_{j=1, j \neq i}^n \alpha_\varepsilon^j \rho_\varepsilon^j \right) - \log \left(\alpha_\varepsilon^i \rho_\varepsilon^i \right) \right) \\ &\leq \int_{B_\delta^i} \frac{\sum_{j=1, j \neq i}^n \alpha_\varepsilon^j \rho_\varepsilon^j}{\alpha_\varepsilon^i} \\ &\leq C \delta^d \varepsilon^{-\frac{d}{2}} e^{-\frac{C(\xi_1 - \delta)^2}{\varepsilon}}, \end{aligned} \quad (3.46)$$

where we used that α_ε^i is bounded below from zero. Hence (3.39) follows directly from (3.40)-(3.46).

Finally, (3.36) follows from combining (3.37), (3.38) and the identity

$$\int \rho_\varepsilon^i(x) \log \rho_\varepsilon^i(x) dx = -\frac{1}{2} \log \left((2\pi\varepsilon)^d \det \Sigma_\varepsilon^i \right) - \frac{d}{2}.$$

□

Remark 3.4.7. *The assumption that $\min_{j \neq i} |m_\varepsilon^i - m_\varepsilon^j| > \xi_2 > 0$ is the crucial condition that allows us to express the entropy of the Gaussian mixture in terms of the mixture of entropies of individual Gaussian (i.e. the equation (3.38)), leading to the asymptotic formula (3.36). Neither formula (3.38) nor (3.23) is likely to be true without such an assumption since the cross entropy terms are not negligible.*

The following corollary immediately follows from Lemma 3.4.6 by plugging in the Laplace approximation of the normalisation constant $Z_{\mu, \varepsilon}$ given in Lemma 3.3.2 and rearranging the terms.

Corollary 3.4.8. *Suppose that $\{(\alpha_\varepsilon, \mathbf{m}_\varepsilon, \Sigma_\varepsilon)\}$ satisfy the same assumption as in Lemma*

3.4.5. If $\limsup_{\varepsilon \downarrow 0} G_\varepsilon(\alpha_\varepsilon, \mathbf{m}_\varepsilon, \Sigma_\varepsilon) < \infty$, then

$$\begin{aligned} G_\varepsilon(\alpha_\varepsilon, \mathbf{m}_\varepsilon, \Sigma_\varepsilon) &= \sum_{i=1}^n \alpha_\varepsilon^i \left(\frac{V_1^\varepsilon(m_\varepsilon^i)}{\varepsilon} + V_2(m_\varepsilon^i) - \frac{d}{2} + \frac{1}{2} \text{Tr}(D^2 V_1^\varepsilon(m_\varepsilon^i) \cdot \Sigma_\varepsilon^i) \right) \\ &+ \sum_{i=1}^n \alpha_\varepsilon^i \left(\log \alpha_\varepsilon^i - \frac{1}{2} \log(\det \Sigma_\varepsilon^i) + \log \left(\sum_{j=1}^n \beta^j \right) \right) + o(1). \end{aligned} \quad (3.47)$$

Remark 3.4.9. Similarly to the discussion in Remark 3.3.9, the residual in (3.47) is here demonstrated to be of order $o(1)$, but the quantitative bound that $|r_\varepsilon| \leq C\varepsilon$ in (3.36) can be used to extract a rate of convergence. This can be used to study the limiting behaviour of posterior measures arising from Bayesian inverse problems when multiple modes are present; see the next section.

3.5 Applications in Bayesian Inverse Problems

Consider the inverse problem of recovering $x \in \mathbf{R}^d$ from the noisy data $y \in \mathbf{R}^d$, where y and x are linked through the equation

$$y = G(x) + \eta. \quad (3.48)$$

Here G is called the forward operator which maps from \mathbf{R}^d into itself, $\eta \in \mathbf{R}^d$ represents the observational noise. We take a Bayesian approach to solving the inverse problem. The main idea is to first model our knowledge about x with a prior probability distribution, leading to a joint distribution on (x, y) once the probabilistic structure on η is defined. We then update the prior based on the observed data y ; specifically we obtain the posterior distribution μ^y which is the conditional distribution of x given y , and is the solution to the Bayesian inverse problem. From this posterior measure one can extract information about the unknown quantity of interest. We remark that since G is non-linear in general, the posterior is generally not Gaussian even when the noise and prior are both assumed to be Gaussian. A systematic treatment of the Bayesian approach to inverse problems may be found in [215].

In Bayesian statistics there is considerable interest in the study of the asymptotic performance of posterior measures from a frequentist perspective; this is often formalised as the *posterior consistency*. To define this precisely, consider a sequence of observations $\{y_j\}_{j \in \mathbf{N}}$, generated from the truth x^\dagger via

$$y_j = G(x^\dagger) + \eta_j, \quad (3.49)$$

where $\{\eta_j\}_{j \in \mathbb{N}}$ is a sequence of random noises. This may model a statistical experiment with increasing amounts of data or with vanishing noise. In either case, posterior consistency refers to concentration of the posterior distribution around the truth as the data quality increases. For parametric statistical models, Doob's consistency theorem [65, Theorem 10.10] guarantees posterior consistency under the identifiability assumption about the forward model. For nonparametric models, in which the parameters of interest lie in infinite dimensional spaces, the corresponding posterior consistency is a much more challenging problem. Schwartz's theorem [13, 208] provides one of the main theoretical tools to prove posterior consistency in infinite dimensional space, which replaces identifiability by a stronger assumption on testability. The posterior contraction rate, quantifying the speed that the posterior contracts to the truth, has been determined in various Bayesian statistical models (see [46, 103, 210]). In the context of the Bayesian inverse problem, the posterior consistency problem has mostly been studied to date for linear inverse problems with Gaussian priors [2, 140]. The recent paper [224] studied posterior consistency for a specific nonlinear Bayesian inverse problem, using the stability estimate of the underlying inverse problem together with posterior consistency results for the Bayesian regression problem.

In this section, our main interest is not in the consistency of posterior distribution, but in characterising in detail its asymptotic behaviour. We will consider two limit processes in (3.49): the small noise limit and the large data limit. In the former case, we assume that the noise $\eta_i = \frac{1}{\sqrt{i}}\eta$ where η is distributed according to the standard normal $N(0, \mathbf{I}_d)$, and we consider the data \mathbf{y}_N given by the most accurate observation, i.e. $\mathbf{y}_N = y_N$. In the later case, the sequence $\{\eta_i\}_{i \in \mathbb{N}}$ is assumed to be independent identically distributed according to the standard normal and we accumulate the observations so that the data $\mathbf{y}_N = \{y_1, y_2, \dots, y_N\}$. In addition, assume that the prior distribution is μ_0 which has the density

$$\mu_0(dx) = \frac{1}{Z_0} e^{-V_0(x)} dx$$

with the normalisation constant $Z_0 > 0$. Since the data and the posterior are fully determined by the noise $\boldsymbol{\eta}$ with $\boldsymbol{\eta} = \eta$ or $\boldsymbol{\eta} = \{\eta_i\}_{i \in \mathbb{N}}$, we denote the posterior by $\mu_N^{\boldsymbol{\eta}}$ to indicate the dependence. By using Bayes' formula, we calculate the posterior distribution for both limiting cases below.

- Small noise limit

$$\begin{aligned}\mu_N^\eta(dx) &= \frac{1}{Z_{N,1}^\eta} \exp\left(-\frac{N}{2} |y_n - G(x)|^2\right) \mu_0(dx) \\ &= \frac{1}{Z_{N,1}^\eta} \exp\left(-\frac{N}{2} \left|G(x^\dagger) - G(x) + \frac{1}{\sqrt{N}}\eta\right|^2\right) \mu_0(dx).\end{aligned}\tag{3.50}$$

- Large data limit

$$\begin{aligned}\mu_N^\eta(dx) &= \frac{1}{Z_{N,2}^\eta} \exp\left(-\frac{1}{2} \sum_{i=1}^N |y_i - G(x)|^2\right) \mu_0(dx) \\ &= \frac{1}{Z_{N,2}^\eta} \exp\left(-\frac{1}{2} \sum_{i=1}^N \left|G(x^\dagger) - G(x) + \eta_i\right|^2\right) \mu_0(dx).\end{aligned}\tag{3.51}$$

In both cases, we are interested in the limiting behaviour of the posterior distribution μ_N^η as $N \rightarrow \infty$. For doing so, we assume the forward operator G satisfies one of the following assumptions.

Assumption 3.5.1. (i) $G \in C^4(\mathbf{R}^d; \mathbf{R}^d)$ and $G(x) = G(x^\dagger)$ implies $x = x^\dagger$. Moreover, G is a C^1 -diffeomorphism in the neighbourhood of x^\dagger .

(ii) $G \in C^4(\mathbf{R}^d; \mathbf{R}^d)$ and the zero set of the equation $G(x) = G(x^\dagger)$ is $\{x_i^\dagger\}_{i=1}^n$. Moreover $x_1^\dagger = x^\dagger$ and G is a C^1 -diffeomorphism in the neighbourhood of x_i^\dagger .

The following model problem gives a concrete example where these assumptions are satisfied.

Model Problem

Consider the following one dimensional elliptic problem

$$\begin{aligned}-u''(x) + \exp(q(x))u(x) &= f(x), \quad x \in (0, 1), \\ u(0) &= u(1) = 0.\end{aligned}\tag{3.52}$$

Here we assume that $q, f \in L^\infty(0, 1)$ and that f is positive on $(0, 1)$. The inverse problem of interest is to find q from the knowledge of the solution u . We restrict ourselves to a finite

dimensional version of (3.52), which comes from the finite difference discretisation

$$-\frac{u_{k+1} - 2u_k + u_{k-1}}{h^2} + e^{q_k} u_k = f_k, \quad k = 1, 2, \dots, M, \quad (3.53)$$

$$u_0 = u_{M+1} = 0.$$

Here u_k , f_k and q_k are approximations to $u(x_k)$, $f(x_k)$ and $q(x_k)$ with $x_k = k/M$, $k = 1, \dots, M$ and $h = 1/(M+1)$. The corresponding finite dimensional inverse problem becomes finding the vector $\mathbf{q} = \{q_k\}_{k=1}^M$ from the solution vector $\mathbf{u} = \{u_k\}_{k=1}^M$ given the right side $\mathbf{f} = \{f_k\}_{k=1}^M$. For ease of notation, let us denote by \mathcal{A} the matrix representation of the one dimensional discrete Laplacian, i.e. $\mathcal{A}_{ii} = 2/h^2$ for $i = 1, 2, \dots, M$ and $\mathcal{A}_{ij} = -1/h^2$ when $|i - j| = 1$. Let \mathcal{Q} be the diagonal matrix with $\mathcal{Q}_{ii} = e^{q_i}$, $i = 1, 2, \dots, M$. With these notations, we can write the forward map G as

$$G : \mathbf{q} \in \mathbf{R}^M \rightarrow \mathbf{u} \in \mathbf{R}^M \quad \mathbf{u} = G(\mathbf{q}) = (\mathcal{A} + \mathcal{Q})^{-1} \mathbf{f}.$$

Note that both \mathcal{A} and \mathcal{Q} are positive definite so that $(\mathcal{A} + \mathcal{Q})$ is invertible. We now discuss this forward map, and variants on it, in relation to Assumption 3.5.1.

First consider Assumption 3.5.1 (i). First, G is smooth in \mathbf{q} since \mathcal{Q} depends smoothly on \mathbf{q} . In particular, for any fixed $\mathbf{q} \in \mathbf{R}^M$ with corresponding solution vector \mathbf{u} , a direct calculation shows that the derivative matrix $D_{\mathbf{q}}G$ of the forward map G is given by

$$D_{\mathbf{q}}G = (\mathcal{A} + \mathcal{Q})^{-1} \mathcal{U} \mathcal{Q}.$$

Here \mathcal{U} is a diagonal matrix with the diagonal vector \mathbf{u} . Due to our assumption that f_k are positive, it follows from the (discrete) maximum principle that the u_k are also positive, which in turn implies that \mathcal{U} is invertible. Consequently, the matrix $D_{\mathbf{q}}G$ is invertible and

$$D_{\mathbf{q}}G^{-1} = \mathcal{Q}^{-1} \mathcal{U}^{-1} (\mathcal{A} + \mathcal{Q}).$$

According to the inverse function theorem, the map $G : \mathbf{R}^M \rightarrow \mathbf{R}^M$ is invertible at every $\mathbf{q} \in \mathbf{R}^M$ and its inverse $G^{-1}(\mathbf{u})$ is smooth in \mathbf{u} . Therefore Assumption 3.5.1 (i) is fulfilled for any $x^\dagger = \mathbf{q}^\dagger \in \mathbf{R}^M$. The problem (3.52) can be modified slightly so that Assumption 3.5.1 (ii) is satisfied. In fact, consider the problem (3.52) with the coefficient $\exp(q)$ replaced by q^2 . Then Assumption 3.5.1 (ii) is satisfied for any $x^\dagger = \mathbf{q}^\dagger$ without zero entries. More specifically, the resulting forward map in this case is still smooth, but the equation $G(\mathbf{q}) = G(\mathbf{q}^\dagger)$ has $n = 2^M$ solutions $\{\mathbf{q}_i^\dagger\}_{i=1}^{2^M}$ corresponding to the fact that \mathbf{q} is only determined up to a sign in each entry. Moreover, if \mathbf{q}^\dagger has no zero entry, G^{-1} is smooth near each of \mathbf{q}_i^\dagger .

We divide our exposition below according to whether the noise is fixed or is considered as a random variable. For a fixed realisation of noise $\boldsymbol{\eta} = \eta$, by applying the theory developed in the previous section, we show the asymptotic normality for μ_N^η in the small noise limit. Furthermore, we obtain a Bernstein-Von Mises type theorem for μ_N^η with respect to both limit processes, small noise and large data.

3.5.1 Asymptotic Normality

In this subsection, we assume that the data is generated from the truth x^\dagger and a single realisation of the Gaussian noise η^\dagger , i.e.

$$y = G(x^\dagger) + \frac{1}{\sqrt{N}}\eta^\dagger.$$

Then the resulting posterior distribution μ_N^η has a density of the form

$$\begin{aligned}\mu_N^\eta(dx) &= \frac{1}{Z_N^\eta} \exp\left(-\frac{N}{2}|y - G(x)|^2 - V_0(x)\right) dx \\ &= \frac{1}{Z_N^\eta} \exp\left(-\frac{N}{2}|G(x^\dagger) - G(x) + \frac{1}{\sqrt{N}}\eta^\dagger|^2 - V_0(x)\right) dx\end{aligned}\tag{3.54}$$

where Z_N^η is the normalisation constant. Notice that μ_N^η has the same form as the measure defined in (3.1) with $\varepsilon = \frac{1}{N}$, $V_1^\varepsilon(x) = V_1^N(x) := \frac{1}{2}|G(x^\dagger) - G(x) + \frac{1}{\sqrt{N}}\eta^\dagger|^2$ and $V_2(x) = V_0(x)$.

Suppose that $V_0 \in C^2(\mathbf{R}^d; \mathbf{R})$ and that G satisfies one of the assumptions in Assumption (3.5.1). Then the potentials V_1^ε and V_2 satisfy Assumption 5.2.1. In particular, we have $V_1^\varepsilon(x) \rightarrow V_1(x) := \frac{1}{2}|G(x^\dagger) - G(x)|^2$ for any $x \in \mathbf{R}^d$ and that $D^2V_1(x_i^\dagger) = DG(x_i^\dagger)^T DG(x_i^\dagger)$. Recall the set of Gaussian measures \mathcal{A} and the set of Gaussian mixtures \mathcal{M}_n and \mathcal{M}_n^ξ (defined in (3.26) and (3.27)). Again, we set $\xi = (\xi_1, \xi_2)$ such that $\xi_1 \in (0, 1)$ and $\min_{i \neq j} |x^i - x^j| \geq \xi_2 > 0$. The following theorem concerning the asymptotic normality of μ_N^η is a direct consequence of Corollary 3.3.4 and Corollary 3.4.4.

Theorem 3.5.2.

- (i) Let $V_0 \in C^2(\mathbf{R}^d; \mathbf{R})$ and G satisfy Assumption 3.5.1 (i). Given any $N \in \mathbb{N}$, let $\nu_N = N(m_N, \frac{1}{N}\Sigma_N) \in \mathcal{A}$ be a minimiser of the functional $\nu \mapsto D_{KL}(\nu || \mu_N^\eta)$ within \mathcal{A} . Then $D_{KL}(\nu_N || \mu_N^\eta) \downarrow 0$ as $N \rightarrow \infty$. Moreover, $m_N \rightarrow x^\dagger$ and $\Sigma_N \rightarrow (DG(x^\dagger)^T DG(x^\dagger))^{-1}$.
- (ii) Let $V_0 \in C^2(\mathbf{R}^d; \mathbf{R})$ and G satisfy Assumption 3.5.1 (ii). Given any $N \in \mathbb{N}$, let $\nu_N \in \mathcal{M}_n^\xi$ be a minimiser of the functional $\nu \mapsto D_{KL}(\nu || \mu_N^\eta)$ within \mathcal{M}_n^ξ . Let $\nu_N = \sum_{i=1}^n \alpha_N^i \nu_N^i$

with $\nu_N^i = N(m_N^i, \frac{1}{N} \Sigma_N^i)$. Then it holds that as $N \rightarrow \infty$

$$m_N^i \rightarrow x_i^\dagger, \Sigma_N^i \rightarrow \left(DG(x_i^\dagger)^T DG(x_i^\dagger) \right)^{-1} \text{ and } \alpha_N^i \rightarrow \frac{\left[\det DG(x_i^\dagger) \right]^{-1} \cdot e^{-V_0(x_i^\dagger)}}{\sum_{j=1}^n \left[\det DG(x_j^\dagger) \right]^{-1} \cdot e^{-V_0(x_j^\dagger)}}.$$

Theorem 3.5.2 (i) states that the measure μ_N^η is asymptotically Gaussian when certain uniqueness and stability properties hold in the inverse problem. Moreover, in this case, the asymptotic Gaussian distribution is fully determined by the truth and the forward map, and is independent of the prior. In the case where the uniqueness fails, but the data only corresponds to a finite number of unknowns, Theorem 3.5.2 (ii) demonstrates that the measure μ_N^η is asymptotically a Gaussian mixture, with each Gaussian mode independent of the prior. However, prior beliefs affect the proportions of the individual Gaussian components within the mixture; more precisely, the un-normalised weights of each Gaussian mode are proportional to the values of the prior evaluated at the corresponding unknowns.

Remark 3.5.3. In general, when $\{\eta_i\}_{i \in \mathbb{N}}$ is a sequence of fixed realisations of the normal distribution, Theorem 3.5.2 does not hold for the measure μ_N^η defined in (3.51) in the large data case. However, we will show that $D_{KL}(\nu_N || \mu_N^\eta)$ will converge to zero in some average sense; see Theorem 3.5.4.

3.5.2 A Bernstein-Von Mises Type Result

The asymptotic Gaussian phenomenon in Theorem 3.5.2 is very much in the same spirit as the celebrated Bernstein-Von Mises (BvM) theorem [65]. This theorem asserts that for a certain class of regular priors, the posterior distribution converges to a Gaussian distribution, independently of the prior, as the sample size tends to infinity. Let us state the Bernstein-Von Mises theorem more precisely in the i.i.d case. Consider observing a set of i.i.d samples $\mathbf{X}^N := \{X^1, X^2, \dots, X^N\}$, where X^i is drawn from distribution P_θ , indexed by an unknown parameter $\theta \in \Theta$. Let P_θ^N be the law of \mathbf{X}^N . Let Π be the prior distribution on θ and denote by $\Pi(\cdot | \mathbf{X}^N)$ the resulting posterior distribution. The Bernstein-Von Mises Theorem is concerned with the behaviour of the posterior $\Pi(\cdot | \mathbf{X}^N)$ under the frequentist assumption that X^i is drawn from some true model P_{θ_0} . A standard finite-dimensional BvM result (see e.g. [65, Theorem 10.1]) states that, under certain conditions on the prior Π and the model P_θ , as $N \rightarrow \infty$

$$d_{TV} \left(\Pi(\theta | \mathbf{X}^N), N \left(\hat{\theta}_N, \frac{1}{N} I_{\theta_0}^{-1} \right) \right) \xrightarrow{P_{\theta_0}^N} 0 \quad (3.55)$$

where $\hat{\theta}_N$ is an efficient estimator for θ , I_θ is the Fisher information matrix of P_θ and d_{TV} represents the total variation distance. As an important consequence of the BvM result, Bayesian credible sets are asymptotically equivalent to frequentist confidence intervals. Moreover, it has been proved that the optimal rate of convergence in the Bernstein-Von Mises theorem is $O(1/\sqrt{N})$; see, for instance, [43, 121]. This means that for any $\delta > 0$, there exists $M = M(\delta) > 0$ such that

$$P_{\theta_0}^N \left(\mathbf{X}^N : d_{TV} \left(\Pi(\theta | \mathbf{X}^N), N \left(\hat{\theta}_N, \frac{1}{N} I_{\theta_0}^{-1} \right) \right) \geq M \frac{1}{\sqrt{N}} \right) \leq \delta. \quad (3.56)$$

Unfortunately, BvM results like (3.55) and (3.56) do not fully generalise to infinite dimensional spaces, see counterexamples in [97]. Regarding the asymptotic frequentist properties of posterior distributions in nonparametric models, various positive results have been obtained recently, see e.g. [46, 47, 103, 140, 145, 210]. For the convergence rate in the nonparametric case, we refer to [46, 103, 210].

In the remainder of the section, we prove a Bernstein-Von Mises type result for the posterior distribution μ_N^η defined by (3.50) and (3.51). If we view the observational noise η and η_i appearing in the data as random variables, then the posterior measures appearing become random probability measures. Furthermore, exploiting the randomness of the η_i , we claim that the posterior distribution in the large data case can be rewritten in the form of the small noise case. Indeed, by completing the square, we can write the expression (3.51) as

$$\mu_N^\eta(dx) = \frac{1}{Z_{N,2}^\eta} \exp \left(-\frac{N}{2} |G(x^\dagger) - G(x) + \frac{1}{N} \sum_{i=1}^N \eta_i|^2 \right) dx. \quad (3.57)$$

Observe that $\mathcal{L} \left(\frac{1}{N} \sum_{i=1}^N \eta_i \right) = \mathcal{L} \left(\frac{1}{\sqrt{N}} \eta \right) = N(0, \frac{1}{N} \mathbf{I}_d)$ due to the normality assumptions on η and η_i . As a consequence it makes no difference which formulation is chosen when one is concerned with the statistical dependence of μ_N^η on the law of η . For this reason, we will only prove the Bernstein-Von Mises result for μ_N^η given directly in the form (3.50).

For notational simplicity, we write the noise level $\sqrt{\varepsilon}$ in place of $\frac{1}{\sqrt{N}}$ and consider random observations $\{y_\varepsilon\}$, generated from a truth x^\dagger and normal noise η , i.e.

$$y_\varepsilon = G(x^\dagger) + \sqrt{\varepsilon} \eta.$$

Given the same prior defined as before, we obtain the posterior distribution

$$\begin{aligned}\mu_\varepsilon^\eta(dx) &= \frac{1}{Z_{\mu,\varepsilon}^\eta} \exp\left(-\frac{1}{2\varepsilon}|y_\varepsilon - G(x)|^2 - V_0(x)\right) dx \\ &= \frac{1}{Z_{\mu,\varepsilon}^\eta} \exp\left(-\frac{1}{2\varepsilon}|G(x^\dagger) - G(x) + \sqrt{\varepsilon}\eta|^2 - V_0(x)\right) dx.\end{aligned}$$

For any fixed η , let ν_ε^η be the best Gaussian measure which minimises the Kullback-Leibler divergence $D_{\text{KL}}(\nu||\mu_\varepsilon^\eta)$ over \mathcal{A} . For ease of calculations, from now on we only consider the rate of convergence under Assumption 3.5.1 (i); the other case can be dealt with in the same manner, see Remark 3.5.8. The main result is as follows.

Theorem 3.5.4. *There exists $C > 0$ such that*

$$\mathbb{E}^\eta D_{\text{KL}}(\nu_\varepsilon^\eta||\mu_\varepsilon^\eta) \leq C\varepsilon \quad (3.58)$$

as $\varepsilon \downarrow 0$.

With the help of Pinsker's inequality (2.1) as well as the Markov inequality, one can derive the following BvM-type result from Theorem 3.5.4.

Corollary 3.5.5. *For any $\delta > 0$, there exists a constant $M = M(\delta) > 0$ such that*

$$\mathbb{P}^\eta\left(\eta : d_{\text{TV}}(\mu_\varepsilon^\eta, \nu_\varepsilon^\eta) \geq M\sqrt{\varepsilon}\right) \leq \delta. \quad (3.59)$$

Remark 3.5.6.

(i) *Because of the statistical equivalence of posterior measures in the limit of large data size and small noise, the posterior measure μ_N^η in the large data case (given by (3.51)) has the same convergence rate as (3.59), namely, for any $\delta > 0$, there exists a constant $M = M(\delta) > 0$ such that*

$$\mathbb{P}^\eta\left(\eta : d_{\text{TV}}(\mu_N^\eta, \nu_N^\eta) \geq M/\sqrt{N}\right) \leq \delta \quad (3.60)$$

as $N \rightarrow \infty$. This recovers the optimal rate of convergence for the posterior as proved for statistical models, see (3.56).

(ii) *For a fixed realisation of the noise η , we have shown in Theorem 3.5.2 (i) that $D_{\text{KL}}(\nu_N||\mu_N^\eta) \downarrow 0$ as $N \rightarrow \infty$. In fact, by following the proof of the Laplace method, one can prove that $D_{\text{KL}}(\nu_N||\mu_N^\eta) = \mathcal{O}(1/\sqrt{N})$. However, we obtain the linear convergence rate in (3.58) (with ε replacing $1/N$) by utilising the symmetric cancellations in the evaluation of Gaussian integrals.*

To prove Theorem 3.5.4, we start with an averaging estimate for the logarithm of the normalisation constant $Z_{\mu,\varepsilon}^\eta$.

Lemma 3.5.7.

$$\mathbb{E}^\eta \log Z_{\mu,\varepsilon}^\eta \leq \frac{d}{2} \log(2\pi\varepsilon) - V_0(x^\dagger) + \log \det DG(x^\dagger) + r_\varepsilon \quad (3.61)$$

where $r_\varepsilon \leq C\varepsilon$ for some $C > 0$ independent of ε .

Proof. Take a constant $\gamma \in (0, \frac{1}{2})$. We write $\mathbb{E}^\eta \log Z_{\mu,\varepsilon}^\eta$ as the sum

$$\mathbb{E}^\eta \log Z_{\mu,\varepsilon}^\eta = \mathbb{E}^\eta (\log Z_{\mu,\varepsilon}^\eta \mathbf{1}_{|\eta| \leq \varepsilon^{-\gamma}}) + \mathbb{E}^\eta (\log Z_{\mu,\varepsilon}^\eta \mathbf{1}_{|\eta| \geq \varepsilon^{-\gamma}}) =: I_1 + I_2.$$

We first find an upper bound for I_2 . By definition,

$$\begin{aligned} Z_{\mu,\varepsilon}^\eta &= \int_{\mathbf{R}^d} \exp \left(-\frac{1}{2\varepsilon} |G(x^\dagger) - G(x) + \sqrt{\varepsilon}\eta|^2 - V_0(x) \right) dx \\ &\leq \int_{\mathbf{R}^d} e^{-V_0(x)} dx = Z_0. \end{aligned}$$

It follows that

$$I_2 \leq \log Z_0 \cdot P^\eta(\eta : |\eta| \geq \varepsilon^{-\gamma}) \leq \log Z_0 \cdot e^{-\varepsilon^{-2\gamma}}.$$

For I_1 , we need to estimate $Z_{\mu,\varepsilon}^\eta$ under the assumption that $|\eta| \leq \varepsilon^{-\gamma}$. Thanks to the condition (i) on G , when $\varepsilon \ll 1$ there exists a unique $m_{\varepsilon,\eta}^\dagger$ such that $G(m_{\varepsilon,\eta}^\dagger) = G(x^\dagger) + \sqrt{\varepsilon}\eta$. Moreover, denoting by H the inverse of G in the neighbourhood of $G(x^\dagger)$, we get from Taylor expansion that

$$m_{\varepsilon,\eta}^\dagger = x^\dagger + DH(G(x^\dagger))\sqrt{\varepsilon}\eta + \varepsilon \sum_{|\alpha|=2} \partial_\alpha H(\xi G(x^\dagger) + (1-\xi)\sqrt{\varepsilon}\eta)\eta^\alpha \quad (3.62)$$

with some $\xi \in (0, 1)$. Thanks to the smoothness assumption on G , the function H is differentiable up to the fourth order and hence the coefficients in the summation are uniformly bounded. Moreover, noting that $DH(G(x^\dagger)) = DG(x^\dagger)^{-1}$, we obtain

$$m_{\varepsilon,\eta}^\dagger = x^\dagger + DG(x^\dagger)^{-1}\sqrt{\varepsilon}\eta + \varepsilon R_\varepsilon(\eta) \quad (3.63)$$

where $\limsup_{\varepsilon \downarrow 0} |R_\varepsilon(\eta)| \leq C|\eta|^2$ for some positive C which is independent of ε and η . Next, according to the proof of Lemma 3.3.2, given any sufficiently small $\delta > 0$, we can write $Z_{\mu,\varepsilon}^\eta = I_\varepsilon^{\delta,\eta} + J_\varepsilon^{\delta,\eta}$ where $|J_\varepsilon^{\delta,\eta}| \leq Ce^{-\frac{C}{\varepsilon}}$ with some $C > 0$ independent of η and

$$I_\varepsilon^{\delta,\eta} = \int_{B_\varepsilon^{\delta,\eta}} \exp \left(-\frac{1}{2\varepsilon} |G(x^\dagger) - G(x) + \sqrt{\varepsilon}\eta|^2 - V_0(x) \right) dx$$

with $B_\varepsilon^{\delta,\eta} := B(m_{\varepsilon,\eta}^\dagger, \delta)$. Now we seek bounds for $I_\varepsilon^{\delta,\eta}$. Thanks to Assumption 3.5.1 (i) and the fact that $m_{\varepsilon,\eta}^\dagger \rightarrow x^\dagger$, G is a C^1 -diffeomorphism in the neighbourhood of $m_{\varepsilon,\eta}^\dagger$. Therefore there exist positive constants $\delta_1 < \delta_2$ depending only on δ such that $B(G(m_{\varepsilon,\eta}^\dagger), \delta_1) \subset G(B_\varepsilon^{\delta,\eta}) \subset B(G(m_{\varepsilon,\eta}^\dagger), \delta_2)$. After applying the transformation $x \mapsto H(x)$ in evaluation of the integral $I_\varepsilon^{\delta,\eta}$, we get

$$\tilde{I}_\varepsilon^{\delta_1,\eta} \leq I_{i,\varepsilon}^{\delta,\eta} \leq \tilde{I}_\varepsilon^{\delta_2,\eta}$$

where

$$\tilde{I}_\varepsilon^{\delta,\eta} := \int_{B(0,\delta)} \exp\left(-\frac{1}{2\varepsilon}|y|^2 - V_0 \circ H(y + G(m_{\varepsilon,\eta}^\dagger))\right) \det(DH(y + G(m_{\varepsilon,\eta}^\dagger))) dy.$$

In order to estimate $\tilde{I}_\varepsilon^{\delta,\eta}$, in $B(0, \delta)$ with some small δ we define two auxiliary functions by setting

$$f_{\varepsilon,\eta}(\cdot) := \exp(-V_0 \circ H(\cdot + G(m_{\varepsilon,\eta}^\dagger))) \det(DH(\cdot + G(m_{\varepsilon,\eta}^\dagger)))$$

and

$$L(\cdot) := \exp(-V_0 \circ H(G(\cdot))) \det(DH(G(\cdot))) = \exp(-V_0(\cdot)) / \det(DG(\cdot)).$$

It is worthy to note that within the ball $B(0, \delta)$, all derivatives up to second order of $f_{\varepsilon,\eta}$ as well as of L can be bounded uniformly with respect to sufficiently small ε and η such that $|\eta| \leq \varepsilon^{-\gamma}$. Taking the equation (3.63) into account, we can expand L near m^\dagger to get that

$$\begin{aligned} f_{\varepsilon,\eta}(0) &= L(m_{\varepsilon,\eta}^\dagger) \\ &= L(x^\dagger) + \nabla L(x^\dagger)^T (m_{\varepsilon,\eta}^\dagger - x^\dagger) + \frac{1}{2} (m_{\varepsilon,\eta}^\dagger - x^\dagger)^T \nabla^2 L(\theta x^\dagger + (1-\theta)m_{\varepsilon,\eta}^\dagger) (m_{\varepsilon,\eta}^\dagger - x^\dagger) \\ &= \frac{\exp(-V_0(x^\dagger))}{\det(DG(x^\dagger))} + \varepsilon^{\frac{1}{2}} \nabla L(x^\dagger)^T DG(x^\dagger)^{-1} \eta + r_{1,\varepsilon,\eta} \end{aligned} \tag{3.64}$$

with some $\theta \in (0, 1)$ and the residual $|r_{1,\varepsilon,\eta}| \leq C\varepsilon|\eta|^2$ for some $C > 0$. Moreover, for any $y \in B(0, \delta)$,

$$f_{\varepsilon,\eta}(y) = f_{\varepsilon,\eta}(0) + \nabla f_{\varepsilon,\eta}(0)^T y + \frac{1}{2} y^T \nabla^2 f_{\varepsilon,\eta}(\xi y) y \tag{3.65}$$

for some $\xi = \xi(y) \in (0, 1)$. Then it follows from (3.64) and (3.65) that

$$\begin{aligned}
\tilde{I}_\varepsilon^{\delta, \eta} &= \int_{B(0, \delta)} \exp\left(-\frac{1}{2\varepsilon}|y|^2\right) f_{\varepsilon, \eta}(y) dy \\
&= \varepsilon^{\frac{d}{2}} \int_{B(0, \varepsilon^{-\frac{1}{2}}\delta)} \exp\left(-\frac{1}{2}|y|^2\right) f_{\varepsilon, \eta}(\varepsilon^{\frac{1}{2}}y) dy \\
&= \varepsilon^{\frac{d}{2}} \left(f_{\varepsilon, \eta}(0) \int_{B(0, \varepsilon^{-\frac{1}{2}}\delta)} \exp\left(-\frac{1}{2}|y|^2\right) dy + \frac{\varepsilon}{2} \int_{B(0, \varepsilon^{-\frac{1}{2}}\delta)} \exp\left(-\frac{1}{2}|y|^2\right) y^T \nabla^2 f_{\varepsilon, \eta}(\xi y) y dy \right) \\
&= (2\pi\varepsilon)^{\frac{d}{2}} \left(\frac{\exp(-V_0(x^\dagger))}{\det(DG(x^\dagger))} + \nabla L(x^\dagger)^T DG(x^\dagger)^{-1} \sqrt{\varepsilon} \eta + r_{2, \varepsilon, \eta} \right)
\end{aligned} \tag{3.66}$$

with $|r_{2, \varepsilon, \eta}| \leq C\varepsilon|\eta|^2$. Notice that the linear term in the expansion (3.65) vanishes from the second line to the third line because the region of integration is symmetric with respect to the origin; the final equality holds because we have counted the exponentially decaying Gaussian integral outside of the ball $B(0, \varepsilon^{-\frac{1}{2}}\delta)$ in the residual $r_{2, \varepsilon, \eta}$. Hence we obtain that for $|\eta| \leq \varepsilon^{-\gamma}$ and ε small enough

$$I_{\varepsilon, \eta}^\delta = (2\pi\varepsilon)^{\frac{d}{2}} \left(\frac{\exp(-V_0(x^\dagger))}{\det(DG(x^\dagger))} + \varepsilon^{\frac{1}{2}} \nabla L(x^\dagger)^T DG(x^\dagger)^{-1} \eta + r_{2, \varepsilon, \eta} \right)$$

with $|r_{2, \varepsilon, \eta}| \leq C\varepsilon|\eta|^2$. As a result, $Z_{\mu, \varepsilon}^\eta$ satisfies the same bound as above. Then by using the Taylor expansion of the log function, one obtains that

$$\log Z_{\mu, \varepsilon}^\eta = \log \left(\frac{(2\pi\varepsilon)^{\frac{d}{2}} \exp(-V_0(x^\dagger))}{\det(DG(x^\dagger))} \right) + \varepsilon^{\frac{1}{2}} p^T \eta + r_{3, \varepsilon, \eta}$$

where p is vector depending only on L, G, V_0 and x^\dagger and $|r_{3, \varepsilon, \eta}| \leq C\varepsilon|\eta|^2$. This implies that when ε is sufficiently small,

$$I_1 = \mathbb{E}^\eta (\log Z_{\mu, \varepsilon}^\eta \mathbf{1}_{|\eta| \leq \varepsilon^{-\gamma}}) = \frac{d}{2} \log(2\pi\varepsilon) - V_0(x^\dagger) + \log \det DG(x^\dagger) + r_\varepsilon.$$

with $|r_\varepsilon| \leq C\varepsilon$. Again the first order term $\varepsilon^{\frac{1}{2}} p^T \eta$ vanishes because of the symmetry of the integration region; the bound $|r_\varepsilon| \leq C\varepsilon$ follows from the bound for $r_{3, \varepsilon, \eta}$ and the Gaussian tail bound. This completes the proof. \square

Proof of Theorem 3.5.4. We prove the theorem by constructing a family of Gaussian measures $\{\bar{\nu}_\varepsilon^\eta\}$ such that

$$\mathbb{E}^\eta D_{\text{KL}}(\bar{\nu}_\varepsilon^\eta || \mu_\varepsilon^\eta) \leq C\varepsilon \tag{3.67}$$

for some $C > 0$. Then the theorem is proved by the optimality of $\nu_{\varepsilon,\eta}$. Recall that $m_{\varepsilon,\eta}^\dagger$ is defined by (3.62). Fixing $\gamma \in (0, \frac{1}{2})$, we define $\bar{\nu}_\varepsilon^\eta = N(\bar{m}_{\varepsilon,\eta}, \bar{\Sigma}_{\varepsilon,\eta})$ with $\bar{m}_{\varepsilon,\eta}$ defined by

$$\bar{m}_{\varepsilon,\eta} = \begin{cases} m_{\varepsilon,\eta}^\dagger & \text{if } |\eta| \leq \varepsilon^{-\gamma}, \\ x^\dagger & \text{otherwise} \end{cases}$$

and that $\bar{\Sigma}_{\varepsilon,\eta} = (DG(\bar{m}_{\varepsilon,\eta})^T DG(\bar{m}_{\varepsilon,\eta}))^{-1}$. Clearly, when ε is small enough, $\bar{m}_{\varepsilon,\eta}$ admits an expansion similar to (3.62). As a consequence, there exist positive constants C_1, c_2, C_2 which are independent of η , such that $\limsup_{\varepsilon \downarrow 0} |\bar{m}_{\varepsilon,\eta}| \leq C_1$ and $c_2 \leq \liminf_{\varepsilon \downarrow 0} \lambda_{\min}(\bar{\Sigma}_{\varepsilon,\eta}) < \limsup_{\varepsilon \downarrow 0} \text{Tr}(\Sigma_\varepsilon) \leq C_2$ hold for all η . With the above choice for $(\bar{m}_{\varepsilon,\eta}, \bar{\Sigma}_{\varepsilon,\eta})$, an application of Lemma 3.3.7 with $V_1^\varepsilon(x) = \frac{1}{2}|G(x^\dagger) - G(x) + \sqrt{\varepsilon}\eta|^2$ and $V_2(x) = V_0(x)$ yields that

$$D_{\text{KL}}(\bar{\nu}_\varepsilon^\eta || \bar{\mu}_\varepsilon^\eta) = V_0(\bar{m}_{\varepsilon,\eta}) - \frac{d}{2} \log(2\pi\varepsilon) + \log \det DG(\bar{m}_{\varepsilon,\eta}) + \log Z_{\mu,\varepsilon}^\eta + r_\varepsilon \quad (3.68)$$

where $r_\varepsilon \leq C\varepsilon$ with $C = C(C_1, c_2, C_2, M_V)$. By the definition of $\bar{m}_{\varepsilon,\eta}$ and the expansion (3.62), it follows from the Taylor expansion for the function $x \mapsto V_0(x) + \frac{1}{2} \log \det DG(x)$ that when $|\eta| \leq \varepsilon^{-\gamma}$ and ε is small enough,

$$V_0(\bar{m}_{\varepsilon,\eta}) + \log \det DG(\bar{m}_{\varepsilon,\eta}) = V_0(x^\dagger) + \log \det DG(x^\dagger) + \sqrt{\varepsilon} q^T \eta + \tilde{r}_{\varepsilon,\eta} \quad (3.69)$$

with some $q \in \mathbf{R}^d$ and $|\tilde{r}_{\varepsilon,\eta}| \leq C\varepsilon$ for some $C > 0$. Then the estimate (3.67) follows, by taking the expectation of (3.68) and using the equation (3.69) and Lemma 3.3.7. \square

Remark 3.5.8. Theorem 3.5.4 proves the rate of convergence with the assumption that G satisfies Assumption 3.5.1 (i). However, the convergence rate remains the same when Assumption 3.5.1 (ii) is fulfilled, and when the best Gaussian measure is replaced by the best Gaussian mixture.

3.5.3 Comparison with Classical BvM Results

We would like to make comparisons between our BvM result for Bayesian inverse problems and classical finite dimensional BvM results for general statistical models [104, 121].

- **Assumption.** In the classical framework of Bayesian inferences, the posterior converges to a Gaussian in the total variation distance (with optimal rate) under the typical assumption that the likelihood function is C^3 and that the Fisher information matrix is non-degenerate; see e.g. [104, Theorem 1.4.2] and [121, Section 4]. The asymptotic covariance of the limiting Gaussian is given by the inverse of the Fisher

information matrix. In the Bayesian inverse problem setting, we improve the convergence to the stronger sense of KL-divergence, but at the expense of requiring higher differentiability (C^4) on the forward map G . Moreover, the matrix product $DG^T DG$ takes the place of the Fisher information matrix in the asymptotic covariance, where DG is invertible because of Assumption 3.5.1.

- **Multimodal Distribution.** The proposed KL-approximation framework allows us to prove the convergence of a multimodal probability measure to a mixture of Gaussian measures. The limiting KL-discrepancy between the target measure and the Gaussian approximation is characterised explicitly as a sum of two relative entropies, see Theorem 3.4.2. In addition, in this case the prior does not disappear in the limit and its influence on the posterior is reflected in the weighted coefficients in the Gaussian mixture. To the best of our knowledge, such results have not been stated in the statistical literature.
- **Proof.** Both our proof and classical proofs for the finite dimensional BvM theorems are essentially based on the local Taylor expansion of the posterior around the truth. But the proofs are carried out in different ways. Classical BvM results in the TV-distance are usually proved by first expanding the posterior density around the maximum likelihood estimator (MLE), which requires tracking the normalisation constant, and then applying the local asymptotic normality of MLE and Le Cam's contiguity arguments to obtain the convergence of the posterior. Our proof, instead, takes advantage of the special formulation of the KL-divergence, i.e. the separation of the normalisation constant from the log density, thereby reducing the convergence proof to establishing precise estimates on the normalisation constant (see Lemma 3.5.7).

3.6 Conclusions

We have studied a methodology widely used in applications, yet little analysed, namely the approximation of a given target measure by a Gaussian, or by a Gaussian mixture. We have employed relative entropy as a measure of goodness of fit. Our theoretical framework demonstrates the existence of minimisers of the variational problem, and studies their asymptotic form in a relevant small parameter limit where the measure concentrates; the small parameter limit is studied by use of tools from Γ -convergence. In the case of a target with asymptotically unimodal distribution the Γ -limit demonstrates perfect reconstruction by the approximate single Gaussian method in the measure concentration limit; and in the case of multiple modes it quantifies the errors resulting from using a single mode fit. Fur-

thermore the Gaussian mixture is shown to overcome the limitations of a single mode fit, in the case of target measure with multiple modes. These ideas are exemplified in the analysis of a Bayesian inverse problem in the small noise or large data set limits, and connections made to the Bernstein-von Mises theory from asymptotic statistics.

The BvM theorem established in this chapter is essentially still parametric. A natural interesting future direction would be to study infinite-dimensional statistical models [106]. In particular it would be interesting to apply our measure approximation approach from Γ -convergence to understand the BvM phenomenon of infinite dimensional non-linear Bayesian inverse problems. In our finite dimensional setting, the inverse problem of interest is essentially well-posed since we assume that both G and DG are invertible, so the only ill-posedness comes from the lack of uniqueness. However, for infinite dimensional inverse problems, the degree of ill-posedness (mild/severe) has a big influence on the precise statement of the BvM theorem. Understanding of this issue requires delicate quantitative stability estimates for the underlying inverse problem. The recent paper [158] proved a BvM result for high dimensional non-linear inverse problems where dimension of the unknown parameter increases with the decreasing noise level. However, it remains an open problem whether the BvM theorem holds for genuinely infinite dimensional non-linear inverse problems. We will address this problem in future work.

Chapter 4

Bayesian Approach to Bar Code Denoising

4.1 Introduction

4.1.1 Background

Barcodes are everywhere in our daily life and are used for in identification for almost all business areas. For example, in supermarkets, most grocery items carry a simple barcode known as the Universal Product Code (UPC). One can check out by simply scanning the UPCs in front of a laser scanner at an automatic machine. In the UPC-A symbology, a (one dimensional) barcode consists of a series of black bars and white spaces above a sequence of 12 numerical digits. There is one-to-one correspondence between these digits and the sequence of black bars and white spaces, and both uniquely determine a barcode. Figure 4.1 presents a typical example of UPC-A barcode. For a detailed description of various barcode symbologies, we refer the interested reader to [183]. In practice, depending on how a barcode is scanned, the barcode signal can be noisy and blurred due to distance, vibrations, etc. Thus a natural question arises: how to reconstruct the original barcode from a noisy signal?

A one dimensional barcode is modelled as a binary function $u : [-1, 1] \rightarrow \{\pm 1\}$. The signal recoded by a scanner is usually modelled as

$$f = G_\sigma * u + n \tag{4.1}$$

where $*$ denotes the convolution operator on $[-1, 1]$, G_σ is a centred Gaussian kernel of variance σ

$$G_\sigma(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{x^2}{2\sigma^2}}.$$



Figure 4.1: An example of UPC-A barcode [131].

More precisely,

$$G_\sigma * u(x) = \int_{-1}^1 G_\sigma(x-y)u(y)dy.$$

The function n represents the random noise. Figure 4.2 provides examples of clean and noisy signals. The Gaussian convolution models the process of blurring. The matter in question becomes an inverse problem of recovering the unknown u given the data f . The mathematical formulation of above barcode inverse problem was firstly set up by Esedoglu [88], where he established the uniqueness of solutions of the inverse problem in the absence of noise. He also analysed a series of minimisation problems based on total variation regularisation and proposed a phase field based numerical algorithm for solving the minimisation problem. The barcode problem can be viewed as a special signal/image processing problem where the signal/image in question is piecewise constant. Hence many image restoration methods can in principle be applied to the barcode problem. Below we briefly review some important previous work on image reconstruction with emphasis on their applications in barcode problems. Generally speaking, most methods discussed in the literature can be classified into two categories: variational and Bayesian.

Total Variation regularisation. The total variation (TV) regularisation method was firstly proposed by Rudin, Osher and Fatemi (ROF) [202] for solving image denoising problems. In the ROF model, the standard Tikhonov regulariser, involving the L^2 -norm of the gradient, is replaced by the TV-norm, that is the L^1 -norm of the gradient. This simple replacement leads to a remarkable improvement in image enhancement, since the TV-based regularisation does not impose strong smoothness constraints and thereby promotes high contrast edges. In the last two decades, TV-based methods have produced enormous impact in modern image processing [40, 49, 50] and a broad range of areas of applied mathematics including compressive sensing [193, 203] and sparse representation [51, 206, 212]. In the context of barcode reconstruction, Esedoglu firstly proposed a blind deconvolution methodology based on the TV-regularisation and considered the minimisation problem of the form

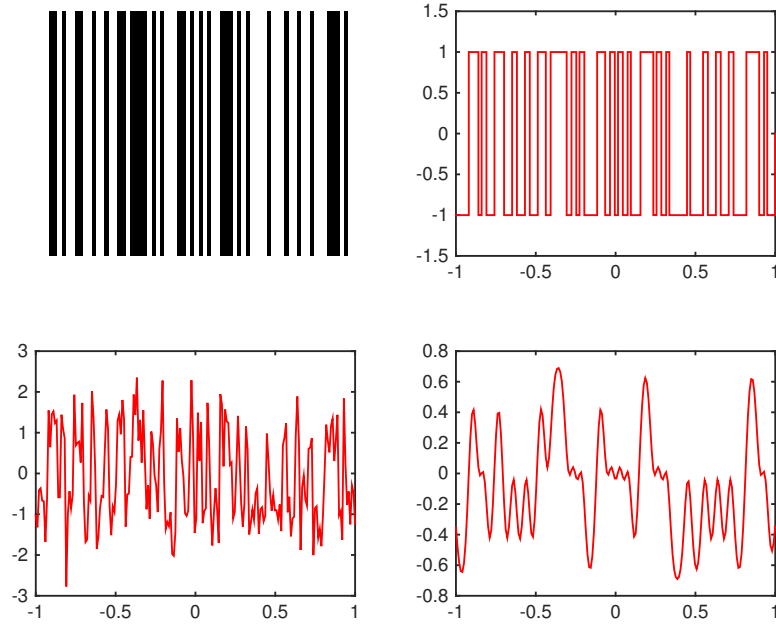


Figure 4.2: Top left: original barcode signal. Top right: clean binary signal. Bottom left: observed signal with additive noise only. Bottom right: observed signal with blurring and additive noise.

$$\inf_{u \in BV((-1,1);\{-1,1\})} \|u\|_{TV} + \lambda \|G_\sigma * u - f\|_{L^2}. \quad (4.2)$$

where total variation semi-norm $\|u\|_{TV} = \int |\nabla u|$ and λ is a weighted constant. The existence of the minimisers of the problem (4.2) and other relevant minimisation problems is established in [88]. Recently, the same variational problem (with σ known a priori) is analysed by Choksi et. al. in [53] and [54] where the authors present sufficient conditions such that the variational problem has a unique minimiser and is given by the original barcode signal.

Phase Field Approach. The phase field method, also known as the diffuse interface method, is usually used as an approximation technique to TV-regularisation and is amenable to numerical computations; see [29, 37, 64]. The idea is to relax the problem (4.2) by replacing the total variational semi-norm by the Ginzburg-Landau functional defined in

(2.3). This leads to the variational problem

$$\inf_{u \in H^1} \int \frac{\varepsilon}{2} |\nabla u(x)|^2 + \frac{1}{\varepsilon} V(u(x)) dx + \lambda \|G_\sigma * u - f\|_{L^2}. \quad (4.3)$$

with V a double well potential taking minimisers $\{\pm 1\}$ and $\varepsilon > 0$. Since the functional of (4.3) is smooth functional in u , the minimisation can be implemented by many numerical algorithms, for example the gradient descent method. The parameter ε controls the thickness of a diffuse interface separating two constant phases $\{u = \pm 1\}$. It can be shown by the standard Γ -convergence theory that a minimiser of (4.3) converges to a minimiser of (4.2) as $\varepsilon \downarrow 0$. Esedoglu and Santosa [89] even derived explicit error bounds for the phase field approximation under some conditions on the blurring width σ , the noise level and the parameter ε . The paper [29] introduced and analysed a convergent iterative scheme for solving the phase field based models for binary recovery.

Beside the approaches discussed above, the Mumford-Shah [174] regularisation and level set methods [37, 179] are another two important methods that have been commonly used in image processing and geometry inversion. We refer to [37, 123, 150, 151, 204, 218, 223] for more details.

Bayesian Approach. The application of Bayesian inference in image restoration has a long history; see early work in [122, 175]. The monograph [230] provides an excellent survey of Bayesian image analysis from a mathematical perspective. In the context of the restoration of blocky images, Calvetti and Somersalo [41, 42] proposed a unified hierarchical Bayesian framework for the purpose of edge-preserving, and they showed how to obtain classical regularisation methods, including the TV-regularisation, from the MAP estimators by careful choices of hyperpriors. However, the models considered in their papers are in discretised form and thus finite dimensional. Helin and Lassas [118] adopted a Bayesian approach for linear inverse problems based on hierarchical Gaussian models and they showed convergence of the MAP estimator to the minimiser of the Mumford-Shah functional as the discretisation parameter tends to infinity. In the recent unpublished note [86], the authors put forward a Bayesian method for recovering piecewise constant signals. With a particular choice of a noise-level-dependent non-Gaussian prior, they show that the resulting MAP estimation is connected to the phase field approach, which in addition is linked to the TV-regularisation in the limit of vanishing noise.

4.1.2 Barcode Problem with Pointwise Observations

In this chapter, we focus our attention on the Bayesian inverse problem of denoising an unblurred barcode signal from a finite number of noisy observations. More precisely, we consider the inverse problem of recovering a function $u : [-1, 1] \rightarrow \{\pm 1\}$ given noisy

observations $\mathbf{f} := \{f_i\}_{i=1}^N$ at sampled locations $\{x_i\}_{i=1}^N \subset (-1, 1)$, where

$$f_i = u(x_i) + \sqrt{\varepsilon}\eta_i. \quad (4.4)$$

Here the noise $\{\eta_i\}_{i=1}^N$ is an independent sequence of Gaussian random variables with each $\eta_i \sim N(0, \sigma_i)$ for some $\sigma_i > 0$. Note that the observed data in (4.4) is finite dimensional, which can be casted into the model (4.1), but only in the extreme case where the convolution kernel becomes a sum of finite number of Diracs. The inverse problem is now under-determined since it has infinite many solutions even when the data is unpolluted by noise ($\varepsilon = 0$).

4.1.3 Purpose

The main purpose of this chapter is to examine the denoising performance of the Bayesian method introduced in [86] for the barcode problem above. More specifically, by choosing a non-Gaussian prior via tilting a Gaussian random field prior with a Ginzburg-Landau type penalty, we obtain a posterior distribution whose MAP estimator is linked to the phase-field formulation to binary reconstruction. Given a specific set of observed data, which is generated from a fixed realisation of noise, we aim to study the limiting behaviour of the posterior conditioning on this specific data. In particular, we identify the Γ -limit of the MAP estimator in the small noise regime and in a simple setting of observations we show that the posterior is concentrated on a set of binary profiles that is determined by the Γ -limit.

4.1.4 Organization

The rest of this chapter is organized as follows. In section 4.2, we present a Bayesian formulation of the inverse problem of barcode denoising. In particular, we define a non-Gaussian prior measure, compute the resulting posterior measure and define the MAP estimator associated to the posterior. Section 4.3.2 is concerned with the Γ -limit of the MAP estimator in the small noise limit. In Section 4.4, we discuss the concentration property of the posterior measure in a simple situation where the data only consists of two measurements. Finally, Section 4.5 is devoted to the proofs of the concentration results.

4.2 Bayesian Formulation of Barcode Denoising

We adopt the Bayesian approach proposed in [86] to the inverse problem of barcode denoising. The key idea is to find the posterior distribution of the unknown function u on the space $C([-1, 1])$ of continuous functions (rather than the space of binary functions), given an appropriate prior and the observed data y .

4.2.1 Prior

We define a prior on $C([-1, 1])$ by tilting a Gaussian bridge measure with an exponential functional which encodes the binary structure of a barcode signal. To be more precise, let $\tilde{\mu}^0$ be the measure of a Brownian bridge starting from -1 at $x = -1$ and hitting 1 at $x = 1$. It is clear that $\tilde{\mu}^0$ is the Gaussian measure on $L^2(-1, 1)$ with mean

$$m_0(x) := x$$

and covariance operator $(-\Delta)^{-1}$ where the inverse is taken with respect to Laplacian with homogeneous Dirichlet boundary condition. Namely $\tilde{\mu}^0 = N(m_0, (-\Delta)^{-1})$. Note that a random function u drawn from $\tilde{\mu}^0$ satisfies the boundary condition $u(\pm 1) = \pm 1$ almost surely.

Let V be the double-well potential

$$V(u) = \frac{1}{4}(1 - u^2)^2.$$

We define the prior measure $\tilde{\mu}_\varepsilon$ via the Radon-Nikodym derivative

$$\tilde{\mu}_\varepsilon(du) \propto \exp\left(-\frac{1}{\varepsilon^2} \int_{-1}^1 V(u(x)) dx\right) \tilde{\mu}^0(du). \quad (4.5)$$

Since $\tilde{\mu}_\varepsilon$ is absolutely continuous with respect to $\tilde{\mu}^0$, it inherits the almost sure properties of $\tilde{\mu}^0$: First a random function u drawn from $\tilde{\mu}_\varepsilon$ is continuous (even Hölder continuous) on $[-1, 1]$; second, u satisfies the boundary conditions $u(\pm 1) = \pm 1$. In addition, the prior measure $\tilde{\mu}_\varepsilon$ produces functions which are close to piecewise constants ± 1 when ε is small; the parameter ε controls the interface width of a transition between -1 and $+1$. We remark that such width parameter can in principle be chosen differently from the parameter ε which indicates the noise level, but we keep the width parameter identical to ε for the purpose of simplifying the limiting process, because our focus is on the asymptotic denoising performance of the Bayesian approach in limits of both small width and vanishing noise.

Observe that the measure $\tilde{\mu}_\varepsilon$ is closely linked to the Ginzburg-Landau energy functional. Indeed, according to Feynman's heuristic interpretation of quantum mechanics [94], the bridge measure $\tilde{\mu}^0$ can be viewed as a Gibbs measure with respect to the kinetic energy, i.e.

$$\tilde{\mu}^0(du) \propto \exp\left(-\frac{1}{2} \int_{-1}^1 |u'(x)|^2 dx\right) du.$$

Feynman's picture is not rigorous since there is no Lebesgue measure du in infinite dimen-

sions. However, this implies that informally the measure $\tilde{\mu}_\varepsilon$ can be interpreted as

$$\begin{aligned}\tilde{\mu}_\varepsilon(du) &\propto \exp\left(-\frac{1}{\varepsilon} \int_{-1}^1 \frac{\varepsilon}{2} |u'(x)|^2 + \frac{1}{\varepsilon} V(u(x)) dx\right) du \\ &\propto \exp\left(-\frac{1}{\varepsilon} E_\varepsilon(u)\right) du\end{aligned}\tag{4.6}$$

where E_ε is the Ginzburg-Landau energy functional defined as (2.3).

4.2.2 Posterior

Recall that the data of the inverse problem is $\mathbf{f} := \{f_i\}_{i=1}^N$ where

$$f_i = u(x_i) + \sqrt{\varepsilon} \eta_i, \quad i = 1, 2, \dots, N.\tag{4.7}$$

The noise $\eta_i \sim N(0, \sigma_i)$ with $\sigma_i > 0$. For the sake of notational convenience, we denote $\lambda_i = 1/(2\sigma_i)$. This gives rise to the likelihood — the condition distribution of $\mathbf{f}|u$, which is a Gaussian distribution on \mathbf{R}^N with the Lebesgue density

$$\rho(\mathbf{f}) = \frac{1}{Z_{\rho, \varepsilon}} \exp\left(-\frac{1}{\varepsilon} \Phi_{\mathbf{f}}(u)\right).$$

Here $\Phi_{\mathbf{f}}(u)$ is the data-misfit functional defined by

$$\Phi_{\mathbf{f}}(u) = \sum_{i=1}^N \lambda_i (u(x_i) - f_i)^2.$$

It follows from the Bayes's rule [215] that the posterior measure is given by

$$\tilde{\nu}_{\varepsilon, \mathbf{f}}(du) = \frac{1}{Z_{\varepsilon, \mathbf{f}}} \exp\left(-\frac{1}{\varepsilon} \Phi_{\mathbf{f}}(u)\right) \tilde{\mu}_\varepsilon(du).\tag{4.8}$$

Note that the pointwise evaluations of u in $\Phi_{\mathbf{f}}(u)$ is well-defined since drawing from $\tilde{\mu}_\varepsilon$ gives continuous functions. In view of the informal interpretation of the measure $\tilde{\mu}_\varepsilon$ (see (4.6)), the posterior measure $\tilde{\nu}_{\varepsilon, \mathbf{f}}$ can be formally written in the form

$$\tilde{\nu}_{\varepsilon, \mathbf{f}}(du) \propto \exp\left(-\frac{1}{\varepsilon} F_\varepsilon(u)\right) du.\tag{4.9}$$

where the functional F_ε is defined by

$$F_{\varepsilon, \mathbf{f}}(u) := E_\varepsilon(u) + \Phi_{\mathbf{f}}(u).\tag{4.10}$$

4.2.3 Scope of the Study

We are interested in the asymptotic behaviour of the posterior measure $\tilde{\nu}_{\varepsilon, \mathbf{f}}$ in the limit $\varepsilon \downarrow 0$. Ideally, from the Bayesian consistency perspective (see (1.2)), one would expect to first view the posterior measure $\tilde{\nu}_{\varepsilon, \mathbf{f}}$ as a random measure (since f is random), and then make statistical statements about the convergence property of the posterior. However, it is not clear to us how to rigorously characterise the stochastic convergence of posterior. Instead, we focus our attention on the study of the asymptotics of $\tilde{\nu}_{\varepsilon, \mathbf{f}}$ conditioning on a fixed realisation of \mathbf{f} . Indeed, to simplify the analysis further, we only consider the data $\mathbf{f} = \{f_i\}_{i=1}^n$ with $f_i \in \{\pm 1\}$. For this specific (and deterministic) choice of \mathbf{f} , we are able to characterise explicitly the asymptotic behaviour of the measure $\tilde{\nu}_{\varepsilon, \mathbf{f}}$ as $\varepsilon \downarrow 0$. Extending the theory to other deterministic observations or allowing random observations is beyond the scope of this chapter.

Since we only treat the specific observed data \mathbf{f} , hereafter for the sake of simplicity of notation, we write the posterior, the data-misfit and the functional $F_{\varepsilon, \mathbf{f}}$ as $\tilde{\nu}_{\varepsilon}$, $\Phi(u)$ and F_{ε} respectively, suppressing their dependence on \mathbf{f} . We would like to investigate the *deterministic concentration* property of the measure $\tilde{\nu}_{\varepsilon}$. In particular, we address the following questions:

- Does the measure $\tilde{\nu}^{\varepsilon}$ concentrate on some limiting set or manifold as $\varepsilon \downarrow 0$ and how to identify it?
- How can we describe the measure concentration phenomenon precisely?

Regarding the first question, the limiting manifold can be guessed from the formulation of $\tilde{\nu}^{\varepsilon}$. In fact, in view of (4.9), when ε is small enough, the measure $\tilde{\nu}^{\varepsilon}$ should formally concentrate around the minimisers of F_{ε} (or equivalently the MAP estimator of $\tilde{\nu}^{\varepsilon}$, see Proposition 4.3.1), whose limits thereby constitute the limiting manifold. We shall identify the limiting manifold with the help of the Γ -convergence of F_{ε} in the next section. Then in Section 4.4, we characterise the concentration of $\tilde{\nu}^{\varepsilon}$ around the limiting manifold more precisely in terms of large deviation inequalities.

4.3 MAP Estimator and its Γ -limit

4.3.1 MAP Estimator

The posterior measure $\tilde{\nu}_{\varepsilon}$ is the solution to the Bayesian inverse problem which contains the updated knowledge about the unknown function u given the data \mathbf{f} . The full probabilistic information of the posterior measure can in principle be retrieved through sampling methods, such as the MCMC methods, but these sampling methods may be prohibitively expensive in

practical computations. The variational approach based on MAP estimator provides a computationally attractive alternative to the sampling approach, leading to a notion of “most likely” function with respect to the posterior measure. The following proposition links the MAP estimator of $\tilde{\nu}_\varepsilon$ to the minimiser of F_ε .

Proposition 4.3.1. *For any fixed $\varepsilon > 0$, the MAP estimator of $\tilde{\nu}_\varepsilon$ exists and is given by the minimiser of the functional F_ε defined (4.10) subject to $u \in H_\pm^1(-1, 1)$.*

Proof. We want to exploit Theorem 2.3.4. First we write the measure $\tilde{\mu}_\varepsilon$ in the form of (2.2). In fact, in view of (4.5) we have

$$\frac{d\tilde{\nu}_\varepsilon}{d\tilde{\mu}^0}(u) \propto \exp(-\Psi(u))$$

with

$$\Psi(u) = \int_{-1}^1 \frac{1}{\varepsilon^2} V(u(x)) dx + \frac{1}{\varepsilon} \Phi(u).$$

In addition, it is easy to check that the functional $\Psi(u) : X = C([-1, 1]) \mapsto \mathbf{R}$ satisfies Assumption 2.3.3. Recall that $\tilde{\mu}^0 = N(m_0, (-\Delta)^{-1})$ with $m_0(x) = x$, which has the Cameron-Martin space $E = H_0^1(-1, 1)$. Then it follows from Theorem 2.3.4 that the MAP estimator $\tilde{\nu}_\varepsilon$ is given by the minimiser of

$$\Psi_{\mathbf{f}}(u) + \frac{1}{2} |u - m_0|_{H^1(-1, 1)}^2$$

subject to

$$u - m_0 \in H_0^1(-1, 1). \tag{4.11}$$

It is clear that the condition (4.11) is equivalent to $u \in H_\pm^1(-1, 1)$. Moreover,

$$|u - m_0|_{H^1(-1, 1)}^2 = |u|_{H^1(-1, 1)}^2 + |m_0|_{H^1(-1, 1)}^2 - 2\langle u', m_0' \rangle_{H^1} = |u|_{H^1(-1, 1)}^2 - 2,$$

where the second equality follows from the boundary condition $u(\pm 1) = \pm 1$. Therefore by the definition of $\Psi(u)$ and $E_\varepsilon(u)$, we can write

$$\begin{aligned} \Psi(u) + \frac{1}{2} |u - m_0|_{H^1(-1, 1)}^2 &= \Psi(u) + \frac{1}{2} |u|_{H^1(-1, 1)}^2 - 1 \\ &= \frac{1}{\varepsilon} (E_\varepsilon(u) + \Phi(u)) - 1. \end{aligned}$$

Finally since multiplying or subtracting a functional by a constant does not affect a minimisation process, it follows that the MAP estimator of $\tilde{\nu}^\varepsilon$ is also identical to the minimiser of F_ε . The proof is complete. \square

Remark 4.3.2. MAP estimator of the posterior \tilde{v}^ε is not unique. In fact, the Γ -limit of F_ε has infinitely many minimisers; see e.g. equation (4.29).

4.3.2 Γ -limit

Recall that the functional

$$\begin{aligned} F_\varepsilon(u) &= E_\varepsilon(u) + \Phi(u) \\ &= \int_{-1}^1 \frac{\varepsilon}{2} |u'(x)|^2 + \frac{1}{\varepsilon} V(u(x)) dx + \sum_{i=1}^N \lambda_i (u(x_i) - f_i)^2. \end{aligned}$$

Remember also that we assumed $f_i \in \{-1, 1\}$ for all $1 \leq i \leq N$. This assumption is essential for proving both the Γ -convergence result of the current section and the measure concentration results in the next section. At first glance, one may guess from the additive structure of F_ε and Proposition 2.4.3 that the Γ -limit of F_ε is the sum of Γ -limit of E_ε (with boundary constraint) and Φ . However, this naive guess turns out to be wrong. This is because the functional $\Phi(u)$ involves pointwise evaluations of u , and hence is not a continuous functional on $L^1(-1, 1)$ which is the space where the Γ -convergence of E_ε takes place. In fact, we shall see that the discontinuity of Φ leads to a different extra cost in the Γ -limit; see Theorem 4.3.5.

Although our Γ -convergence result of the functional F_ε does not follow directly from that of E_ε , their proofs rely substantially on the same trick by Modica-Mortola [171]. Since this trick plays a crucial role in many subsequent proofs, we briefly review it now. The Modica-Mortola trick uses the simple arithmetic inequality $a^2 + b^2 \geq 2ab$ to obtain an estimate for the minimal energy cost:

$$\begin{aligned} & \liminf_{\varepsilon \rightarrow 0} \inf_u \left\{ E_\varepsilon(u) \mid u(\pm 1) = \pm 1 \right\} \\ &= \liminf_{\varepsilon \rightarrow 0} \inf_u \left\{ \int_{-1}^1 \frac{\varepsilon}{2} |u'(x)|^2 + \frac{1}{\varepsilon} V(u(x)) dx \mid u(\pm 1) = \pm 1 \right\} \\ &= \inf_u \left\{ \int_{-\infty}^{\infty} \frac{1}{2} |u'(x)|^2 + V(u(x)) dx \mid u(\pm \infty) = \pm 1 \right\} \\ &\geq \inf_u \left\{ \int_{-\infty}^{\infty} |\sqrt{2V(u(x))} u'(x)| dx \mid u(\pm \infty) = \pm 1 \right\} \\ &= \int_{-1}^1 \sqrt{2V(u(x))} dx =: c_0. \end{aligned} \tag{4.12}$$

Furthermore, the minimal energy cost is achieved when the inequality of above becomes equality, i.e.

$$|u'(x)| = |\sqrt{2V(u(x))}|.$$

With the choice $V = \frac{1}{4}(1 - u^2)^2$ and the boundary constraint $u(\pm\infty) = \pm 1$, there exists a strictly increasing function such that

$$u'(x) = \sqrt{2V(u(x))}.$$

In fact, by adding the intermediate condition $u(0) = 0$, one obtains that $u(x) = \tanh(x/\sqrt{2})$. It is important to notice that the minimiser u converges to ± 1 exponentially as $x \rightarrow \pm\infty$.

To identify the Γ -limit of F_ε , we first prove a lower bound for the local energy associated to F_ε in the simple case that the data consists of a single observation only. To be more precise, let $I = (s, t)$ be a subinterval on $(-1, 1)$ and let $r \in (s, t)$ be a fixed intermediate point. Fix also constants $\lambda > 0$ and $f \in \{-1, 1\}$. We define the localised energy functional

$$\overline{F}_{\varepsilon, \lambda}(u) := \int_s^t \frac{\varepsilon}{2} |u'(x)|^2 + \frac{1}{\varepsilon} V(u(x)) dx + \lambda(u(r) - f)^2. \quad (4.13)$$

It is clear that the unique global minimiser of $\overline{F}_{\varepsilon, \lambda}(u)$ is the constant profile $u \equiv f$, since we assumed that $f \in \{-1, 1\}$. However, the situation is different if we minimise F_ε subject to the boundary constraint $u(s) = u(t) = -f$. In fact, under such conditions, the Ginzburg-Landau energy favours the profile $u \equiv -f$ while the energy of the data-fidelity part pushes the profile to be close to $u \equiv f$. The next lemma demonstrates that the competition between these two energy terms (weighted by the constant λ) leads to a non-constant optimal profile which incurs strictly less energy cost than the constant profiles.

Lemma 4.3.3. *Let $\overline{F}_{\varepsilon, \lambda}(u)$ be given by (4.13) with $\lambda > 0$, $f \in \{-1, 1\}$ and $V(u) = \frac{1}{4}(1 - u^2)^2$. Then it holds that*

$$\liminf_{\varepsilon \rightarrow 0} \inf_u \{\overline{F}_{\varepsilon, \lambda}(u) \mid u(s) = u(t) = -f\} = \rho_\lambda := \min_{h \in \mathbf{R}} \rho(h) \quad (4.14)$$

where

$$\rho(h) = 2 \int_{1-h}^1 \sqrt{2V(u)} du + \lambda(2 - h)^2, \quad h \in \mathbf{R}. \quad (4.15)$$

In particular, the minima ρ_λ is attained at $h^* = \sqrt{2}\lambda \wedge 2$.

Proof. We only consider the case that $f = -1$ since the opposite case can be treated similarly. In this case, the energy cost of the constant function $u \equiv 1$ is 4λ . We look for a non-constant optimal profile which incurs lower energy cost. Obviously the value $u(r)$ is the key parameter to be tuned to achieve that and we set $u(r) = 1 - h$. Firstly observe that it is impossible to obtain a lower energy cost than 4λ when $h \leq 0$. In fact, for $h \geq 0$ or

equivalently $u(r) \leq 1$, $\overline{F}_{\varepsilon, \lambda}(u) \geq \lambda(2-h)^2 \geq 4\lambda$.

Next we consider the case that $0 < h < 2$. We first claim that

$$\begin{aligned} & \inf_u \left\{ \int_s^t \frac{\varepsilon}{2} |u'(x)|^2 + \frac{1}{\varepsilon} V(u(x)) dx \mid u(s) = u(t) = 1 \text{ and } u(r) = 1-h \right\} \\ &= 2 \int_{1-h}^1 \sqrt{2V(u)} du + o(1)_{\varepsilon \downarrow 0} \end{aligned}$$

when ε sufficiently small. In fact, first by the elementary arithmetic inequality, we have

$$\begin{aligned} & \inf_u \left\{ \int_s^t \frac{\varepsilon}{2} |u'(x)|^2 + \frac{1}{\varepsilon} V(u(x)) dx \mid u(s) = u(t) = 1 \text{ and } u(r) = 1-h \right\} \\ & \geq 2 \int_{1-h}^1 \sqrt{2V(u)} du. \end{aligned}$$

Then we build a test function \overline{u}_ε to match the lower bound. For doing this, similar to the Modica-Mortola trick we construct v_ε solving the problem

$$v'_\varepsilon(x) = \text{sign}(x-r) \cdot \sqrt{2V(v_\varepsilon(x))}/\varepsilon \text{ on } (s, t) \quad \text{and} \quad v_\varepsilon(r) = 1-h.$$

The above differential equation has an explicit solution

$$v_\varepsilon(x) = \frac{\frac{2-h}{h} \exp(2|x-r|/\varepsilon) - 1}{\frac{2-h}{h} \exp(2|x-r|/\varepsilon) + 1},$$

from which one can see that v_ε is exponentially close to 1 at the end points s and t when $\varepsilon \ll 1$; see Figure 4.3. Then we build \overline{u}_ε by setting it to be v_ε on $[s+\delta, t-\delta]$ for some small δ and by linearly interpolating from its value at $s+\delta$ to 1 at s and from its value at $t-\delta$ to 1 at t respectively. Thanks to the exponential convergence of \overline{u}_ε to 1 near s and t , the energy on $(s, s+\delta)$ and $(t-\delta, t)$ is $o(1)_{\varepsilon \downarrow 0}$. It follows that

$$\begin{aligned} & \inf_u \left\{ \int_s^t \frac{\varepsilon}{2} |u'(x)|^2 + \frac{1}{\varepsilon} V(u(x)) dx \mid u(s) = u(t) = 1 \text{ and } u(r) = 1-h \right\} \\ & \leq \int_s^t \frac{\varepsilon}{2} |\overline{u}'_\varepsilon(x)|^2 + \frac{1}{\varepsilon} V(\overline{u}_\varepsilon(x)) dx \\ & = \int_{1-h}^{\overline{u}_\varepsilon(s+\delta)} \sqrt{2V(u)} du + \int_{1-h}^{\overline{u}_\varepsilon(t-\delta)} \sqrt{2V(u)} du + \int_{(s, s+\delta) \cup (t-\delta, t)} \frac{\varepsilon}{2} |\overline{u}'_\varepsilon(x)|^2 + \frac{1}{\varepsilon} V(\overline{u}_\varepsilon(x)) dx \\ & = 2 \int_{1-h}^1 \sqrt{2V(u)} du + o(1)_{\varepsilon \downarrow 0}, \end{aligned}$$

where in the last equality we have again used the exponential convergence of \overline{u}_ε to 1 near s and t .

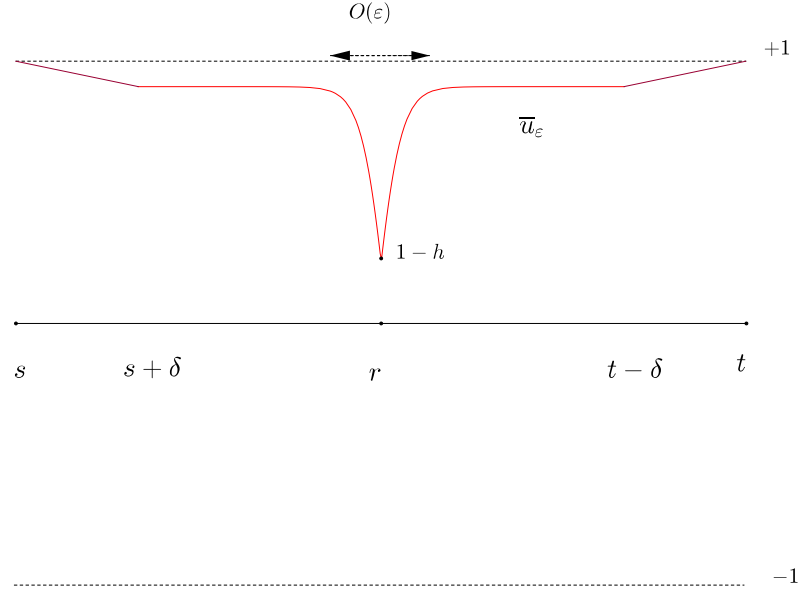


Figure 4.3: The optimal profile \bar{u}_ε .

Taking account of the extra cost from the data-misfit, that is $\lambda(2 - h)^2$, we obtain that

$$\inf_u \{ \bar{F}_{\varepsilon, \lambda}(u) \mid u(s) = u(t) = 1 \text{ and } u(r) = 1 - h \} \leq \rho(h) + o(1)_{\varepsilon \downarrow 0}.$$

Now we proceed further by optimizing $\rho(h)$. With $V(u) = \frac{1}{4}(1 - u^2)^2$,

$$\rho(h) = 2 \int_{1-h}^1 \sqrt{2V(u)} du + \lambda(2 - h)^2 = \frac{\sqrt{2}}{3}(3h^2 - h^3) + \lambda(2 - h)^2, \quad h \in (0, 2).$$

Taking the derivative of above, one obtains

$$\rho'(h) = -\sqrt{2}(h - 2)(h - \sqrt{2}\lambda).$$

Consequently, (i) if $0 < \lambda < \sqrt{2}$ then ρ decreases in $(0, \sqrt{2}\lambda)$ and increases in $(\sqrt{2}\lambda, 2)$ so that the optimal value of h is given by $h^* = \sqrt{2}\lambda$ and $\rho(h^*) < \min(4\lambda, 2c_0)$; (ii) if $\lambda \geq \sqrt{2}$ then ρ is a decreasing function in $(0, 2)$ and hence the minimiser $h^* = 2$ which gives $\rho(h^*) = 2c_0$.

Finally, when $h \geq 2$, it is easy to see from Modica-Mortola trick that the energy cost is larger than $2c_0$.

In conclusion, we have obtained that

$$\inf_u \{ \bar{F}_{\varepsilon, \lambda}(u) \mid u(s) = u(t) = 1 \} \leq \rho(h^*) + o(\varepsilon).$$

The proof is complete by letting $\varepsilon \rightarrow 0$. \square

Remark 4.3.4. We emphasise that both the minimum value ρ_λ and the minimiser h^* depend on the weight λ .

Now we are ready to prove the Γ -convergence result of F_ε . To state the main result, we need a bit of notation. Recall the set of observational points $\{x_n\}_{n=1}^N$ and the data $\mathbf{f} = \{f_n\}_{n=1}^N$. Given a function $u \in BV((-1, 1); \{-1, 1\})$, we denote by $S(u)$ the jump set of u . We define the set $B_n \subset BV((-1, 1); \{-1, 1\})$ associated to an observational point x_n by

$$B_n = \{u \in BV((-1, 1); \{-1, 1\}) \mid x_n \notin S(u) \text{ and } u(x_n) = -f_n\}.$$

Observe that a function $u \in B_n$ has no jump at x_n and takes opposite sign to the measurement f_n at x_n . Define the one-sided limits $u(t^\pm) = \lim_{s \downarrow 0} u(t \pm s)$.

The following theorem identifies the Γ -limit of F_ε .

Theorem 4.3.5. *The Γ -limit of F_ε with respect to $L^1(-1, 1)$ is*

$$F(u) = \begin{cases} c_0 \#S(u) + c_0 \frac{1+u((-1)^+)}{2} + c_0 \frac{1-u(1^-)}{2} \\ \quad + \sum_{n=1}^N \rho_{\lambda_n} \mathbf{1}_{B_n}(u) & u \in BV((-1, 1); \{-1, 1\}) \\ +\infty & \text{otherwise} \end{cases} \quad (4.16)$$

Remark 4.3.6. *The Γ -limit above consists of three parts: The first part (the first term) gives the energy cost caused by the internal jumps of u ; the second part (the second and the third term) is responsible for the energy costs coming from the boundary constraints $u_\varepsilon(\pm 1) = \pm 1$, which increases by c_0 for each violation of boundary condition since u takes values in $\{1, -1\}$; the third part (the last term) accounts for the extra cost induced by the data-misfit.*

Proof. We first prove the lower bound inequality, i.e. if $u_\varepsilon \rightarrow u$ in $L^1(-1, 1)$ with $u_\varepsilon \in H_{\pm}^1(-1, 1)$ and $u \in L^1(-1, 1)$, then $F(u) \leq \liminf_\varepsilon F_\varepsilon(u_\varepsilon)$. Assume that $\liminf_\varepsilon F_\varepsilon(u_\varepsilon) < \infty$ otherwise there is nothing to prove. Let $\{F_{\varepsilon_k}\}$ be a subsequence of $\{F_\varepsilon\}$ such that $\lim_{k \rightarrow \infty} F_{\varepsilon_k}(u_{\varepsilon_k}) = \liminf_\varepsilon F_\varepsilon(u_\varepsilon) < \infty$. Then it also holds that $\lim_{k \rightarrow \infty} E_{\varepsilon_k}(u_{\varepsilon_k}) < \infty$. In addition, we have that $u \in BV((-1, 1); \{-1, 1\})$ because of the compactness of E_ε (see Lemma 6.2 in [25]). Since $u_{\varepsilon_k} \rightarrow u$ in $L^1(-1, 1)$, by extracting a further subsequence, without being relabelled, we can assume that $u_{\varepsilon_k} \rightarrow u$ a.e.

To proceed, we need to introduce a few more notations. Recall the observational points $\{x_i\}_{i=1}^N$ and let the jump set of u be give by $S(u) = \{y_j\}_{j=1}^J$ with $J = \#S(u)$.

Given an interval $I \subset (-1, 1)$, we denote by $E_\varepsilon(u; I)$ the energy $E_\varepsilon(u)$ restricted on I . Similarly, we define

$$F_\varepsilon(u; I) = E_\varepsilon(u; I) + \sum_{n=1}^N \lambda_n (u(x_n) - f_n)^2 \mathbf{1}_{\{x_n \in I\}}$$

Let $\#S(u; I)$ represent the number of jumps of u on I .

Let $-1 = z_0 < z_1 < \dots < z_{M-1} < z_M = 1$ be a partition of $(-1, 1)$ such that the leftmost and rightmost subintervals contain no x_i or y_j and that each interval subinterval (z_i, z_{i+1}) , $i = 0, \dots, M-1$ does not contain x_i or y_j . By definition u is continuous at z_i . It is also clear that $M \leq J + N + 2$ and the inequality holds whenever one of the jumps coincides with one of measurement points, namely $x_{i_0} = y_{j_0}$ for some i_0 and j_0 . Denote by \mathcal{J} the index set of the subintervals containing only one jump of u without measurement points, by \mathcal{I} the index set of the subintervals containing one jump which coincides with some measurement point, and by \mathcal{M} the index set of the subintervals containing only one measurement without jumps. Then we have

$$(-1, 1) = (z_0, z_1) \cup \left(\bigcup_{i \in \mathcal{J} \cup \mathcal{I} \cup \mathcal{M}} (z_i, z_{i+1}) \right) \cup (z_{M-1}, z_M).$$

Moreover, it is trivial that

$$\#\mathcal{J} + \#\mathcal{I} = \#S(u) = J \quad \text{and} \quad \#\mathcal{I} + \#\mathcal{M} = N. \quad (4.17)$$

Now we calculate the lower bound of the localised energy of $F_{\varepsilon_k}(u_{\varepsilon_k})$ on a fixed subinterval (z_i, z_{i+1}) . Without loss of generality, we assume that as $k \rightarrow \infty$,

$$u_{\varepsilon_k}(z_i) \rightarrow u(z_i) \quad \text{for all } i = 1, \dots, M-1. \quad (4.18)$$

We start by considering the energy on the leftmost subinterval (z_0, z_1) . Since it contains no jumps of u or measurements, $F_{\varepsilon_k}(u_{\varepsilon_k}; (z_0, z_1)) = E_{\varepsilon_k}(u_{\varepsilon_k}; (z_0, z_1))$. If $u \equiv -1$ on (z_0, z_1) , then it is clear that $\lim_{k \rightarrow \infty} F_{\varepsilon_k}(u_{\varepsilon_k}; (z_0, z_1)) = 0$ since $u_{\varepsilon_k} \rightarrow u = -1$ a.e. on (z_0, z_1) . On the contrary, if $u \equiv 1$, then due to the boundary condition $u_{\varepsilon_k}(z_0) = -1$ and the assumption that $u_{\varepsilon_k} \rightarrow u$ a.e., we can obtain by the trick of Modica-Mortola that

$$\lim_{k \rightarrow \infty} F_{\varepsilon_k}(u_{\varepsilon_k}; (z_0, z_1)) = \lim_{k \rightarrow \infty} E_{\varepsilon_k}(u_{\varepsilon_k}; (z_0, z_1)) \geq c_0.$$

In summary, we have

$$\lim_{k \rightarrow \infty} F_{\varepsilon_k}(u_{\varepsilon_k}; (z_0, z_1)) \geq c_0 \frac{1 + u((-1)^+)}{2}. \quad (4.19)$$

Similarly on the rightmost subinterval, it holds that

$$\lim_{k \rightarrow \infty} F_{\varepsilon_k}(u_{\varepsilon_k}; (z_{M-1}, z_M)) \geq c_0 \frac{1 - u(1^-)}{2}. \quad (4.20)$$

Next we consider a subinterval (z_i, z_{i+1}) with $i \in \mathcal{J} \cup \mathcal{I}$, in which u has only one jump. By the assumption (4.18) we know that u_{ε_k} exhibits a transition layer between -1 and 1 on (z_i, z_{i+1}) . As a consequence,

$$\lim_{k \rightarrow \infty} F_{\varepsilon_k}(u_{\varepsilon_k}; (z_i, z_{i+1})) \geq \lim_{k \rightarrow \infty} E_{\varepsilon_k}(u_{\varepsilon_k}; (z_i, z_{i+1})) \geq c_0 \#S(u; (z_i, z_{i+1})) = c_0 \quad (4.21)$$

On the interval (z_i, z_{i+1}) with $i \in \mathcal{M}$, u has no jumps and hence we pay zero cost for the Ginzburg-Landau component in F_{ε_k} . However, there is a measurement, denoted by f_{n_i} , at some point $x_{n_i} \in (z_i, z_{i+1})$, which may incur an energy cost for the data-misfit. In fact, if $u \equiv f_{n_i}$ on (z_i, z_{i+1}) , then we do not pay extra cost for the data-misfit, but if $u \equiv -f_{n_i}$ on (z_i, z_{i+1}) , or equivalently $u \in B_{n_i}$, then it follows from Lemma 4.3.3 that we pay at least ρ_λ for the total energy. Therefore, for $i \in \mathcal{M}$, we have obtained that

$$\lim_{k \rightarrow \infty} F_{\varepsilon_k}(u_{\varepsilon_k}; (z_i, z_{i+1})) \geq \rho_{\lambda_i} \mathbf{1}_{B_{n_i}}(u). \quad (4.22)$$

Finally, by summing over the subintervals, we get from (4.19)-(4.22) that

$$\begin{aligned} \lim_{k \rightarrow \infty} F_{\varepsilon_k}(u_{\varepsilon_k}) &= \lim_{k \rightarrow \infty} \sum_i F_{\varepsilon_k}(u_{\varepsilon_k}; (z_i, z_{i+1})) \\ &\geq \sum_{i \in \mathcal{J} \cup \mathcal{I}} c_0 \#S(u; (z_i, z_{i+1})) + c_0 \frac{1 + u((-1)^+)}{2} + c_0 \frac{1 - u(1^-)}{2} + \sum_{i \in \mathcal{M}} \rho_{\lambda_i} \mathbf{1}_{B_{n_i}}(u) \\ &= c_0 \#S(u) + c_0 \frac{1 + u((-1)^+)}{2} + c_0 \frac{1 - u(1^-)}{2} + \sum_{n=1}^N \rho_{\lambda_n} \mathbf{1}_{B_n}(u) \end{aligned}$$

where in the last equality we have used (4.17) and the fact that $B_{n_i} = \emptyset$ if $i \notin \mathcal{M}$. This proves the desired lower bound inequality.

For the upper bound inequality, it suffices to prove the following: given a function $u \in BV((-1, 1); \{-1, 1\})$ and any fixed small constant $\eta > 0$, there exists a recovery sequence $u_\varepsilon \rightarrow u$ in $L^1(-1, 1)$ such that $\limsup_\varepsilon F_\varepsilon(u_\varepsilon) \leq F(u) + \eta$. Let $\cup_{i=0}^{M-1} (z_i, z_{i+1})$ be the same partition as used in proving the lower bound inequality. Remember that u is continuous at internal partition points. This allows us to construct the recovery sequence by

first defining it piecewisely in subintervals and then gluing the individual pieces together. First on the leftmost or the rightmost subinterval, by the same arguments used for the lower bound inequality one can construct a recovery sequence $\{u_\varepsilon\}$, which are either flat or “tanh-like”, such that

$$\limsup_{\varepsilon} F_\varepsilon(u_\varepsilon; (z_0, z_1)) \leq c_0 \frac{1 + u((-1)^+)}{2} + \eta \quad (4.23)$$

and that

$$\limsup_{\varepsilon} F_\varepsilon(u_\varepsilon; (z_{M-1}, z_M)) \leq c_0 \frac{1 + u(1^-)}{2} + \eta. \quad (4.24)$$

Next consider a subinterval (z_i, z_{i+1}) with $i \in \mathcal{J}$. On such an interval, since there is no measurement and u has one jump, one can use the Modica-Mortola trick to obtain a “tanh-like” function u_ε satisfying

$$F_\varepsilon(u_\varepsilon; (z_i, z_{i+1})) = E_\varepsilon(u_\varepsilon; (z_i, z_{i+1})) \leq c_0 + \eta/M \quad (4.25)$$

for ε small enough.

Furthermore, for (z_i, z_{i+1}) with $i \in \mathcal{I}$, we divide our discussion into two cases according to the value of u at the jump point x_{n_i} : (i) u fits with the data on the left of x_{n_i} , i.e. $u(x_{n_i}^-) = f_{n_i}, u(x_{n_i}^+) = -f_{n_i}$; (ii) u fits with the data on the right of x_{n_i} , i.e. $u(x_{n_i}^-) = -f_{n_i}, u(x_{n_i}^+) = f_{n_i}$. In both cases, one can define a recovery sequence u_ε on (z_i, z_{i+1}) by shifting the sequence obtained by Modica-Mortola’s method to the left or right of x_{n_i} by a distance of order $\mathcal{O}(\varepsilon)$. See the illustration in Figure 4.3.2. By doing so, we have $u_\varepsilon \rightarrow u$ in $L^1(-1, 1)$ and that $u_\varepsilon(x_{n_i}) \rightarrow f_{n_i}$. As a result,

$$F_\varepsilon(u_\varepsilon; (z_i, z_{i+1})) = E_\varepsilon(u_\varepsilon; (z_i, z_{i+1})) + \lambda_{n_i}(u(x_{n_i}) - f_{n_i})^2 \leq c_0 + \eta/M \quad (4.26)$$

for ε small enough.

Finally, consider the interval (z_i, z_{i+1}) with $i \in \mathcal{M}$, in which the data f_{n_i} is measured at x_{n_i} . If $u \equiv f_{n_i}$ a.e. on (z_i, z_{i+1}) , then choosing $u_\varepsilon \equiv f_{n_i}$ gives zero total energy cost. On the contrary, if $u \equiv -f_{n_i}$ so that $u \in B_{n_i}$, then we can choose a recovery sequence u_ε similar to the test function defined in Lemma 4.3.3 so that

$$F_\varepsilon(u_\varepsilon; (z_i, z_{i+1})) \leq \rho_{\lambda_i} + o(1)_{\varepsilon \downarrow 0}.$$

In conclusion, we have

$$F_\varepsilon(u_\varepsilon; (z_i, z_{i+1})) \leq \rho_{\lambda_i} \mathbf{1}_{B_{n_i}}(u) + \eta/M. \quad (4.27)$$

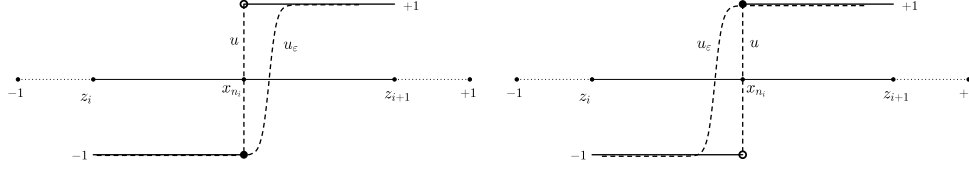


Figure 4.4: u_ε and u on (z_i, z_{i+1}) with $i \in \mathcal{I}$.

Now we obtain a global recovery sequence u_ε by simply concatenating the sequence in individual subintervals. Moreover, it follows from the estimates (4.23)-(4.27) and the equality (4.17) that

$$\begin{aligned} \limsup_{\varepsilon \rightarrow 0} F_\varepsilon(u_\varepsilon) &= \limsup_{\varepsilon \rightarrow 0} \sum_{i=0}^{M-1} F_\varepsilon(u_\varepsilon; (z_i, z_{i+1})) \\ &\leq c_0 \# S(u) + \sum_{n=1}^N \rho_{\lambda_n} \mathbf{1}_{B_n}(u) + \eta \leq F(u) + \eta. \end{aligned}$$

The proof is now complete. \square

4.4 Concentration of $\tilde{\nu}_\varepsilon$

In this section, we study the concentration phenomenon of the posterior measure $\tilde{\nu}^\varepsilon$ defined by (4.8). Again we emphasise that this concentration property is *deterministic* since $\tilde{\nu}^\varepsilon$ is a conditional posterior measure given the special observation \mathbf{f} with $f_i \in \{\pm 1\}$. The intuitive discussion in the end of Section 4.2 already suggests that the measure $\tilde{\nu}^\varepsilon$ should concentrate on the set of the minimisers of the Γ -limit F . Our aim of this section is to make this more precise. For doing this, we will restrict our attention to the case where the minimisers of F can be determined explicitly. In fact, although the minimisation of F is taken only over the space of binary functions, the structure of a minimiser in \mathcal{M} can still be quite complicated; in particular, the number of jumps of the minimiser is only determined implicitly by the parameters λ_n, x_n, f_n . Therefore, for simplicity, we shall focus on a simple situation where the data is composed of only two observations f_\pm at $x_\pm \in (-1, 1)$ with $x_- < x_+$:

$$f_\pm = u(x_\pm) + \sqrt{\varepsilon} \eta_\pm$$

with η_{\pm} distributed according to the same Gaussian distribution $N(0, \sigma)$. Moreover, to simplify our analysis further, we also assume that $f_{\pm} \in \{-1, 1\}$. Under these assumptions, the posterior measure is

$$\tilde{\nu}^{\varepsilon}(du) = \frac{1}{Z_{\varepsilon}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_{\varepsilon}(du) \quad (4.28)$$

where Z_{ε} is the normalisation constant and

$$\Phi(u) = \lambda((u(x_-) - f_-)^2 + (u(x_+) - f_+)^2)$$

with $\lambda = 1/(2\sigma)$. From Feynman's interpretation of $\tilde{\mu}^{\varepsilon}$ (cf. equation (4.6)), we have informally

$$\tilde{\nu}^{\varepsilon}(du) \propto \exp\left(-\frac{1}{\varepsilon}F_{\varepsilon}(u)\right) du$$

with $F_{\varepsilon}(u) = E_{\varepsilon}(u) + \Phi(u)$.

According to Theorem 4.3.5, the Γ -limit of F_{ε} is given by

$$F(u) = \begin{cases} c_0 \# S(u) + c_0 \frac{1+u((-1)^+)}{2} + c_0 \frac{1-u(1^-)}{2} \\ \quad + \rho_{\lambda} (\mathbf{1}_{B_-}(u) + \mathbf{1}_{B_+}(u)) & \text{if } u \in BV((-1, 1); \{-1, 1\}), \\ +\infty & \text{otherwise,} \end{cases}$$

where $B_{\pm} = \{u \in BV((-1, 1); \{-1, 1\}) \mid x_{\pm} \notin S(u) \text{ and } u(x_{\pm}) = -f_{\pm}\}$. According to the choices of f_{\pm} , we identify the set of the minimisers of F explicitly in two different cases:

- Case (I): $f_- = -1$ and $f_+ = 1$. The set of minimisers of F is

$$\mathcal{M}_-^+ := \{-\mathbf{1}_{[-1, \xi)} + \mathbf{1}_{[\xi, 1]} \mid \xi \in [x_-, x_+]\}. \quad (4.29)$$

In fact, it is not hard to see that the first three terms of F are minimised when $u \in \mathcal{M} \cup \{\pm \mathbf{1}_{[-1, 1]}\}$ where

$$\mathcal{M} := \{-\mathbf{1}_{[-1, \xi)} + \mathbf{1}_{[\xi, 1]} \mid \xi \in [-1, 1]\} \quad (4.30)$$

and the resulting minimum value is c_0 . Additionally, the final term vanishes if $u \in \mathcal{M}_-^+$ but induces a cost of ρ_{λ} when $u \in \mathcal{M} \cup \{\pm \mathbf{1}_{[-1, 1]}\} \setminus \mathcal{M}_-^+$.

- Case (II): $f_- = 1$ and $f_+ = -1$. In this case, the minimum of F depends crucially on the value of λ . If λ is small, then the measured data has less influence on the

energy and hence leads to optimal profiles with a single transition, which only match the boundary constraints. However, if λ is large, then the data becomes informative enough so that the optimal profiles could exhibit three transitions fitting perfectly with the data. To characterise this more precisely, let us define the set

$$\overline{\mathcal{M}} := \left\{ -\mathbf{1}_{[-1, \xi_1)} + \mathbf{1}_{[\xi_1, \xi_2)} - \mathbf{1}_{[\xi_2, \xi_3)} + \mathbf{1}_{[\xi_3, 1]} \mid \xi_1 \in [-1, x_-], \right. \\ \left. \xi_2 \in [x_-, x_+) \text{ and } \xi_3 \in [x_+, 1] \right\}.$$

Then one can show by direct calculations that the set of minimiser of F is

$$\mathcal{M}_\lambda := \begin{cases} \mathcal{M} \setminus \mathcal{M}^\pm & 0 < \lambda < \sqrt{2}, \\ (\mathcal{M} \setminus \mathcal{M}^\pm) \cup \overline{\mathcal{M}} & \lambda = \sqrt{2}, \\ \overline{\mathcal{M}} & \lambda > \sqrt{2}. \end{cases} \quad (4.31)$$

We now state our main results in the following theorems that show that the posterior $\tilde{\nu}_\varepsilon$ concentrates around the L^2 -neighbourhood of the optimal manifolds \mathcal{M}_\pm^\pm and \mathcal{M}_λ in case (I) and case (II) respectively.

Theorem 4.4.1. *Let the data be given as in Case (I). There exists $\delta_0 > 0$ such that when $\delta \leq \delta_0$ the following holds: There exists $\varepsilon_0 > 0$ and $C(\delta) > 0$ such that when $\varepsilon \leq \varepsilon_0$*

$$\tilde{\nu}_\varepsilon \left(\text{dist}_{L^2(-1,1)}(u, \mathcal{M}_\pm^\pm) \geq \delta \right) \leq \exp \left(-\frac{C(\delta)}{\varepsilon} \right).$$

Theorem 4.4.2. *Let the data be given as in Case (II). There exists $\delta_0 > 0$ such that when $\delta \leq \delta_0$ the following holds: There exists $\varepsilon_0 > 0$ and $C(\delta) > 0$ such that when $\varepsilon \leq \varepsilon_0$*

$$\tilde{\nu}_\varepsilon \left(\text{dist}_{L^2(-1,1)}(u, \mathcal{M}_\lambda) \geq \delta \right) \leq \exp \left(-\frac{C(\delta)}{\varepsilon} \right).$$

Remark 4.4.3. *We shall see from the proofs of above theorems that the constant $C(\delta) \sim \mathcal{O}(\delta^2)$ when $\delta \ll 1$.*

In our proofs, we will rarely deal with the posterior measure $\tilde{\nu}_\varepsilon$ itself, but will mostly work with its rescaled counterpart. More specifically, let us introduce the scaling operator

$$T_\varepsilon : L^2(-1, 1) \rightarrow L^2(-\varepsilon^{-1}, \varepsilon^{-1}) \quad (T_\varepsilon u)(\cdot) = u(\varepsilon \cdot).$$

This allows us to define a series of push-forward measures: $\nu_\varepsilon = T_\varepsilon^* \tilde{\nu}_\varepsilon$, $\mu^\varepsilon = T_\varepsilon^* \tilde{\mu}_\varepsilon$ and $\mu_\varepsilon^0 = T_\varepsilon^* \mu_0$. By the definition (4.5), the measure μ_ε is absolutely continuous with respect

to the Gaussian measure μ_ε^0 with the Radon-Nikodym derivative

$$\frac{d\mu_\varepsilon}{d\mu_\varepsilon^0}(u) \propto \exp\left(-\frac{1}{\varepsilon} \int_{-\varepsilon^{-1}}^{\varepsilon^{-1}} V(u(x))dx\right)$$

where μ_ε^0 is the distribution of a Brownian bridge process on $[-\varepsilon^{-1}, \varepsilon^{-1}]$ connecting ± 1 with variance ε . In Feynman's picture the measure μ_ε can be interpreted as

$$\mu_\varepsilon(du) \propto \exp\left(-\frac{1}{\varepsilon} \int_{-\varepsilon^{-1}}^{\varepsilon^{-1}} \left(\frac{1}{2}|u'(x)|^2 + V(u(x))\right)dx\right) du. \quad (4.32)$$

Furthermore, according to (4.28) the measure ν_ε is given by

$$\nu_\varepsilon(du) = \frac{1}{Z_\varepsilon} \exp\left(-\frac{1}{\varepsilon} \Phi_\varepsilon(u)\right) \mu_\varepsilon(du),$$

where the functional Φ_ε is defined by

$$\Phi_\varepsilon(u) = \lambda \left((u(x_-/\varepsilon) - f_-)^2 + u(x_+/\varepsilon) - f_+ \right)^2. \quad (4.33)$$

It is important to observe that the normalisation constant Z_ε above is unchanged in the scaling transformation.

In [229], a similar concentration result to ours was proved for the measure μ_ε defined in (4.32), whereas the system size considered there is of order $\mathcal{O}(\varepsilon^{-\gamma})$ with $\gamma < 2/3$. In particular, it is shown that the measure concentrates around the minimisers of the Ginzburg-Landau energy functional on the whole line, i.e.

$$\int_{-\infty}^{\infty} \frac{1}{2} |u'(x)|^2 + V(u(x)) dx$$

subject to the boundary conditions $u(\pm\infty) = \pm 1$. Moreover, on the original interval $[-1, 1]$, the sequence of measures $\tilde{\mu}_\varepsilon$ converges to a limit $\tilde{\mu}$ which concentrates on the set \mathcal{M} defined in (4.30). Recently, Otto et al. [180] studied the measure μ_ε in the context of system sizes that grow exponentially with respect to the inverse noise up to certain critical exponential size determined by the minimum energy cost c_0 . They mainly focus on the competition between the energy and the entropic effect on the measure that emerges due to the large system size. One of their main results is that the probability of finding $2n + 1$ transitions scales like $L_\varepsilon^{2n} \exp(-\frac{2nc_0}{\varepsilon})$ where L_ε represents the system size. As a consequence, it is most likely that the system exhibits only one transition layer. Furthermore, it is also shown in [180] that the location of the single transition layer is uniform distributed when the system size grows at least logarithmically with respect to inverse noise. The key

idea of proving these results [180] is to decompose the measure of interest, which is defined on a growing interval, into a collection of conditional measures that are defined on order-one subintervals on which the large deviation principle applies. Additional important ingredients such as Markov properties and reflection arguments help to assemble the large deviation estimates on the subintervals into the ultimate estimate on the whole interval. We shall adopt the similar arguments to prove our main concentration results in the next section.

4.5 Proofs of Concentration Results

Since our concentration results for the posterior measure $\tilde{\mu}^\varepsilon$ are based on some preliminary results about the measures μ_ε established in [180], we first recall these results in the next subsection. The proofs of Theorem 4.4.1 and Theorem 4.4.2 are then given in Section 4.5.2 and Section 4.5.3 respectively.

4.5.1 Preliminaries

Definition 4.5.1 (Up/down transition layers). *Given a subinterval (x_-, x_+) on the real line, we say that u has an up transition layer on (x_-, x_+) if*

$$u(x_\pm) = \pm 1 \quad \text{and} \quad |u(x)| < 1 \quad \text{for all } x \in (x_-, x_+).$$

We say that u has a down transition layer on (x_-, x_+) if the same condition holds with signs reversed, and that u has a transition layer if it has an up or down transition layer.

Definition 4.5.2 (γ^- transition layers). *Fix $\gamma \in (0, 1/2)$ and suppose $x_- < x_+$. We say that u has a γ^- up transition layer on (x_-, x_+) if*

$$u(x_\pm) = \pm(1 - \gamma) \quad \text{and} \quad |u(x)| < 1 - \gamma \quad \text{for all } x \in (x_-, x_+).$$

We say that u has a γ^- down transition layer on (x_-, x_+) if the same condition holds with signs reversed, and that u has a γ^- transition layer if it has a γ^- up or a γ^- down transition layer.

Recall from (4.12) that the minimum Ginzburg-Landau energy cost of one transition layer is

$$c_0 = \int_{-1}^1 \sqrt{2V(u)} du.$$

The following theorem provides an upper bound for the probability of the occurrence of multiple γ^- transition layers.

Theorem 4.5.3. [180, Theorem 1.5] For every $n \in \mathbb{N}$, any $\eta > 0$ sufficiently small and some sufficiently small $\gamma > 0$, there exists $\varepsilon_0 > 0$ such that for $\varepsilon \leq \varepsilon_0$, one has the upper bound

$$\mu_\varepsilon(u \text{ has } (2n+1)\gamma^- \text{ transition layers}) \lesssim \varepsilon^{-2n} \exp\left(-\frac{2nc_0 - \eta}{\varepsilon}\right). \quad (4.34)$$

Theorem 4.5.3 implies that there is a high probability for the system to have only one transition layer. In addition, the next theorem shows that the layer location is uniformly distributed.

Theorem 4.5.4. [180, Theorem 1.9] Let $d_\varepsilon > 0$ be such that

$$|\log \varepsilon| \ll d_\varepsilon \leq \varepsilon^{-1}.$$

Then for any x such that $[x - d_\varepsilon, x + d_\varepsilon] \subset [-\varepsilon^{-1}, \varepsilon^{-1}]$, we have

$$\frac{1}{\varepsilon d_\varepsilon} \mu_\varepsilon(\text{there is an up layer contained in } [x - d_\varepsilon, x + d_\varepsilon]) \approx 1. \quad (4.35)$$

The proofs of above theorems are based on a sequence of deterministic and probabilistic lemmas. We recall some of these lemmas below since they will also be important ingredients in the proof of our main results. To state the lemmas, we need a few notations. Let u be a random function distributed according to μ_ε . We denote by $\mu_{\varepsilon, (x_-, x_+)}^{u_-, u_+}$ the law of paths u on (x_-, x_+) conditioned on the boundary conditions $u(x_\pm) = u_\pm$. Let $\mathbb{E}_{(x_-, x_+)}^{\mu_\varepsilon, u_-, u_+}$ be the corresponding expectation under the measure $\mu_{\varepsilon, (x_-, x_+)}^{u_-, u_+}$. Given a function $u \in H^1(x_-, x_+)$, we define

$$E_{(x_-, x_+)}(u) := \int_{x_-}^{x_+} \left(\frac{1}{2} (\partial_x u)^2 + V(u(x)) \right) dx.$$

Let \mathcal{A}^{bc} be the set of continuous paths u on $[x_-, x_+]$ that satisfy $u(x_\pm) = u_\pm$. For any subset $\mathcal{A} \subset \mathcal{A}^{\text{bc}}$, we define the energy difference $\Delta E(\mathcal{A})$ by

$$\Delta E(\mathcal{A}) := \inf_{u \in \mathcal{A}} E_{(x_-, x_+)}(u) - \inf_{u \in \mathcal{A}^{\text{bc}}} E_{(x_-, x_+)}(u). \quad (4.36)$$

We denote by $I_{x_\pm}^{u_\pm}$ the minimal kinetic energy, that is the Gaussian part of the energy of the linear interpolation based on the nodes x_\pm and data u_\pm :

$$I_{x_\pm}^{u_\pm} = \frac{(u_+ - u_-)^2}{2(x_+ - x_-)}.$$

We also define the δ -neighbourhood of a set \mathcal{A} by

$$B(\mathcal{A}, \delta) = \{u \mid \exists v \in \mathcal{A} \text{ such that } \|v - u\|_\infty \leq \delta\}.$$

The following two lemmas provide uniform large deviation estimates for the conditional measure $\mu_{\varepsilon, (x_-, x_+)}^{u_-, u_+}$, which will be used repeatedly in our proofs.

Lemma 4.5.5. [180, Proposition 3.4] Fix constants $1 < M, R < \infty$ and $0 < \ell_- < \ell_+ < \infty$. For any $x_\pm \in \mathbf{R}$ with $x_+ - x_- \in [\ell_-, \ell_+]$ and any $u_\pm \in [-M, M]$, let \mathcal{A} be a measurable subset of $C([x_-, x_+])$ consisting of paths u that satisfy the boundary conditions $u(x_\pm) = u_\pm$. Additionally, assume that

$$\inf_{u \in \mathcal{A}} E_{(x_-, x_+)}(u) - I_{x_\pm}^{u_\pm} \leq R. \quad (4.37)$$

Then for any $\delta, \gamma > 0$ there exists an ε_0 such that for all $\varepsilon \leq \varepsilon_0$ we have

$$\mu_{\varepsilon, (x_-, x_+)}^{u_-, u_+}(\mathcal{A}) \leq \exp\left(-\frac{1}{\varepsilon}(\Delta E(B(\mathcal{A}, \delta)) - \gamma)\right),$$

where ΔE is defined in (4.36). This ε_0 depends on M, R, ℓ_\pm, δ , and γ but not on the particular choice of x_\pm, u_\pm . It only depends on the set \mathcal{A} through the choice of R in condition (4.37).

Lemma 4.5.6. [180, Proposition 3.5] Fix constants M and $0 < \ell_- < \ell_+ < \infty$. Suppose that $\ell = x_+ - x_- \in [\ell_-, \ell_+]$ and $u_\pm \in [-M, M]$. Assume that there exists an energy minimiser

$$u_* = \operatorname{argmin}_{u \in \mathcal{A}} E_{(x_-, x_+)}(u)$$

satisfying $u_* \in [-M, M]$. Then, for any $\delta, \gamma > 0$ small enough, there exists an ε_0 such that for all $\varepsilon \leq \varepsilon_0$ we have

$$\mu_{\varepsilon, (x_-, x_+)}^{u_-, u_+}(\mathcal{A}) \geq \exp\left(-\frac{1}{\varepsilon}(\Delta E(\mathcal{A}) + \gamma)\right),$$

where ΔE is defined in (4.36). This ε_0 depends on M, R, ℓ_\pm, δ , and γ but not on the particular choice of x_\pm, u_\pm .

We also recall a two-sided strong Markov property from [180] for the measure $\mu_{\varepsilon, (x_-, x_+)}^{u_-, u_+}$. This Markov property will play an important role in the proof of Theorem 4.4.2. To make it precise, suppose that $[\hat{x}_-, \hat{x}_+] \subset [x_-, x_+]$. Given a fixed path $\mathbf{u} \in C([x_-, x_+])$, we say u is distributed according to $\mu_{\varepsilon, (\hat{x}_-, \hat{x}_+)}^{\mathbf{u}}$ if it coincides with \mathbf{u} outside of $[x_-, x_+]$ almost surely and is distributed according to $\mu_{\varepsilon, (x_-, x_+)}^{\mathbf{u}(\hat{x}_-), \mathbf{u}(\hat{x}_+)}$ on $[\hat{x}_-, \hat{x}_+]$. Given left and right

stopping points χ_{\pm} , we define the σ -algebra $\mathcal{F}_{[x_-, \chi_-]}$ of events that occur to the left of χ_- and the σ -algebra $\mathcal{F}_{[\chi_+, x_+]}$ of events that occur to the right of χ_+ by

$$\begin{aligned}\mathcal{F}_{x_-, \chi_-} &:= \{\mathcal{A} \in \mathcal{F}_{x_-, x_+} : \forall x \quad \mathcal{A} \cap \{\chi_- \leq x\} \in \mathcal{F}_{x_-, x}\}, \\ \mathcal{F}_{\chi_+, x_+} &:= \{\mathcal{A} \in \mathcal{F}_{x_-, x_+} : \forall x \quad \mathcal{A} \cap \{\chi_+ \geq x\} \in \mathcal{F}_{x, x_+}\}.\end{aligned}$$

The strong Markov property is stated in the following lemma.

Lemma 4.5.7. *[180, Lemma 3.3] Suppose that χ_- and χ_+ are left and right stopping points with $\chi_- < \chi_+$ almost surely. Suppose that $\Phi : C([x_-, x_+]) \rightarrow \mathbf{R}$ is measurable and bounded. Then for any $u_{\pm} \in \mathbf{R}$, we have*

$$\mathbb{E}_{(x_-, x_+)}^{\mu_{\varepsilon}, u_-, u_+}(\Phi \mid \mathcal{F}_{[x_-, \chi_-]}, \mathcal{F}_{[\chi_+, x_+]}) = \mathbb{E}_{\chi_-, \chi_+}^{\mu_{\varepsilon}, \mathbf{u}}(\Phi).$$

The next two lemmas state that two particular events are very unlikely to happen under the measure μ_{ε} : the event that the transition exhibits an extremely large excursion, and the event that the transition takes place over an extremely long sub-interval.

Lemma 4.5.8. *[180, Lemma 4.1] There exists $M_1 \in (0, \infty)$, $C \in (0, \infty)$ (depending only on V) such that the following holds. For any $M \geq M_1$, there exists $\varepsilon_0 > 0$ such that for all $\varepsilon \leq \varepsilon_0$ and any x_0 in $(-\varepsilon^{-1}, \varepsilon^{-1})$ there holds*

$$\mu_{\varepsilon}(|u(x_0)| \geq M) \leq \exp\left(-\frac{M}{\varepsilon C}\right).$$

Lemma 4.5.9 (Long transitions). *[180, Lemma 2.3] There exists $C < \infty$ (depending only on V) such that, for any $M \in (0, \infty)$ and any small $\gamma \in (0, 1/2)$, there exist ℓ_* and ε_0 with the following property: for any $\ell \geq \ell_*$ and any $\varepsilon \leq \varepsilon_0$, there holds*

$$\mu_{\varepsilon, (-2\ell, 2\ell)}^{u_-, u_+}(|u(x)| < 1 - \gamma \text{ on all of } [-\ell, \ell] \text{ and } u(\pm 2\ell) = u_{\pm}) \leq \exp\left(-\frac{\gamma^2 \ell}{C\varepsilon}\right)$$

for all $u_{\pm} \in [-M, M]$.

4.5.2 Proof of Theorem 4.4.1

For any $\delta > 0$, we define the event

$$\mathcal{A}^{\delta} := \{u : \text{dist}_{L^2(-1, 1)}(u, \mathcal{M}_-^+) \geq \delta\}.$$

By (4.28), the probability of this event under the measure $\tilde{\nu}_\varepsilon$ is

$$\tilde{\nu}_\varepsilon(\mathcal{A}^\delta) = \frac{1}{Z_\varepsilon} \int_{\mathcal{A}^\delta} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du). \quad (4.38)$$

We prove Theorem 4.4.1 by establishing a lower bound for the normalisation constant Z_ε (cf. Theorem 4.5.11) and an upper bound for the integral in (4.38) (cf. Theorem 4.5.13). To that end, it is crucial to understand the order of smallness of the following small parameters: δ, η, γ and ε . Remember that γ comes from γ -transition layers introduced in Definition 4.5.2. The small parameter η will appear in the estimate on the normalisation constant Z_ε ; see e.g. Theorem 4.5.11. The rule is as follows: given a small positive δ , we first choose η and γ such that

$$\gamma \ll \eta \ll \delta. \quad (4.39)$$

Then the parameter ε is chosen to be small enough according to the previous three parameters.

Now we divide the interval $[-\varepsilon^{-1}, \varepsilon^{-1}]$ into $2N_\varepsilon$ subintervals with $N_\varepsilon := \lfloor \frac{1}{\varepsilon\ell} \rfloor$ where ℓ is a sufficiently large constant (but is still of order one), which is to be specified later. Denote by

$$x_{\pm k} := \begin{cases} \pm k\ell, & k = 0, \dots, (N_\varepsilon - 1), \\ \pm \varepsilon^{-1}, & k = \pm N_\varepsilon \end{cases} \quad (4.40)$$

the endpoints of subintervals. Without loss of generality, we can assume that x_\pm/ε belong to the set of endpoints and that $x_-/\varepsilon = x_{k_-}, x_+/\varepsilon = x_{k_+}$. Consider the overlapping intervals

$$I_k := [x_{k-1}, x_{k+1}] \quad \text{for } k = -(N_\varepsilon - 1), \dots, (N_\varepsilon - 1).$$

Note that $x_{\pm N_\varepsilon}$ is separated from $x_{\pm(N_\varepsilon-1)}$ by up to length 2ℓ , while the rest of the points are separated by length ℓ .

We use Y to denote a generic sub-interval of $(-\varepsilon^{-1}, \varepsilon^{-1})$ which may vary from occasion to occasion. For a small ε and a large ℓ , we denote by $x_{k_1} = k_1\ell$ and $x_{k_2} = k_2\ell$ two endpoints to the left and to the right of Y respectively with distance ℓ from Y . For this

Y and a large constant $M > 0$, we define the following sets

$$\begin{aligned}
\mathcal{A}_1 &:= \{u : \exists k \in \{-(N_\varepsilon - 1), \dots, (N_\varepsilon - 1) : |u(x_k)| \geq M\}\}, \\
\mathcal{J}_Y &:= \{u \in \mathcal{A}_1^c : u \text{ has one } \gamma^- \text{ up layer of length } \leq 2\ell \text{ in } Y\}, \\
\mathcal{J}_{Y,3}^- &:= \{u \in \mathcal{J}_Y : \text{there exists } x \leq (k_1 - 1)\ell \text{ with } u(x) \geq 1 - \gamma\}, \\
\mathcal{J}_{Y,3}^+ &:= \{u \in \mathcal{J}_Y : \text{there exists } x \leq (k_2 + 1)\ell \text{ with } u(x) \leq -1 + \gamma\}, \\
\mathcal{J}_{Y,3} &= \mathcal{J}_{Y,3}^- \cup \mathcal{J}_{Y,3}^+.
\end{aligned} \tag{4.41}$$

We remark that $\mathcal{J}_{Y,3}^-$ (or $\mathcal{J}_{Y,3}^+$) is an empty set if $x_{k_1} < -1$ (or $x_{k_2} > 1$). We use the subscript “3” to indicate that every path in $\mathcal{J}_{Y,3}^\pm$ contains at least three γ -transition layers. The following lemma (cf. [180, Lemma 5.4]) states that the probability of having extra layers is exponentially smaller than the probability of having only a single transition layer.

Lemma 4.5.10. *Fix any sufficiently small $\eta > 0$ and large $M > 0$. For any $\gamma > 0$ sufficiently small and $\ell < \infty$ sufficiently large, there exists ε_0 such that for $\varepsilon \leq \varepsilon_0$ we have*

$$\mu_\varepsilon(\mathcal{J}_{Y,3}) \lesssim \exp\left(-\frac{2c_0 - \eta}{\varepsilon}\right). \tag{4.42}$$

Now we are ready to prove a lower bound on the normalisation constant Z_ε . For doing so, we set $Y = (x_-/(2\varepsilon) + 4\ell, x_+/(2\varepsilon) - 4\ell)$ and assume that $Y \subset (x_-/\varepsilon, x_+/\varepsilon)$. We also denote

$$\varphi_{\pm 1}(u) := \left| \int_u^{\pm 1} \sqrt{2V(s)} ds \right|. \tag{4.43}$$

Theorem 4.5.11. *For any small $\eta > 0$, there exists $\varepsilon_0 > 0$ such that when $\varepsilon \leq \varepsilon_0$,*

$$Z_\varepsilon \gtrsim \exp\left(-\frac{\eta}{\varepsilon}\right). \tag{4.44}$$

Proof. For any $\eta > 0$, we have that

$$\begin{aligned}
Z_\varepsilon &= \int \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \\
&= \int \exp\left(-\frac{1}{\varepsilon}\Phi_\varepsilon(u)\right) \mu_\varepsilon(du) \\
&\geq \exp\left(-\frac{2\lambda\eta^2}{\varepsilon}\right) \mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_\pm}) \mp 1| \leq \eta).
\end{aligned} \tag{4.45}$$

Then the theorem is proved if we can show that there exists a constant $\tilde{C} > 0$ such that for

all $\varepsilon \leq \varepsilon_0$

$$\mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_\pm}) \mp 1| \leq \eta) \geq \tilde{C}. \quad (4.46)$$

Now we prove (4.46) in two steps.

Step 1. We claim that when $\varepsilon \ll 1$, $\mu_\varepsilon(\mathcal{J}_Y \setminus \mathcal{J}_{Y,3}) \geq \tilde{C}$ for some positive \tilde{C} . In fact, it follows from Lemma 4.5.8, Theorem 4.5.4 and the definition of Y that

$$\begin{aligned} \mu_\varepsilon(\mathcal{J}_Y) &= \mu_\varepsilon\{u \text{ has one } \gamma^- \text{ up layer of length } \leq 2\ell \text{ in } Y\} - \mu_\varepsilon(\mathcal{A}_1) \\ &\geq \frac{x_+ - x_-}{4} - \exp\left(-\frac{M}{\varepsilon C}\right). \end{aligned}$$

This together with Lemma 4.5.10 implies that

$$\mu_\varepsilon(\mathcal{J}_Y \setminus \mathcal{J}_{Y,3}) \geq \frac{x_+ - x_-}{4} - \exp\left(-\frac{M}{\varepsilon C}\right) - \exp\left(-\frac{2c_0 - \eta}{\varepsilon}\right) \geq \frac{x_+ - x_-}{8},$$

when $\varepsilon \ll 1$.

Step 2. The following estimates holds: There exists a constant $C(\eta) > 0$ such that when $\varepsilon \ll 1$,

$$\mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_+}) - 1| \geq \eta) \leq \exp\left(-\frac{C(\eta)}{\varepsilon}\right), \quad (4.47)$$

and

$$\mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_-}) + 1| \geq \eta) \leq \exp\left(-\frac{C(\eta)}{\varepsilon}\right). \quad (4.48)$$

Here we only give the proof of (4.47) since (4.48) can be dealt with in the same manner. First by the definition of \mathcal{J}_Y and $\mathcal{J}_{Y,3}$, it is easy to see the following inclusion holds:

$$\begin{aligned} \{u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_+}) - 1| \geq \eta\} &\subset \{u : |u(x_{k_+-2})| \leq M, |u(x_{k_++2})| \leq M, \\ &u(x) \geq -1 + \gamma \text{ for all } x \in [x_{k_+-1}, x_{k_++1}], |u(x_{k_+}) - 1| \geq \eta\}. \end{aligned}$$

Consequently, we have

$$\begin{aligned} \mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_-}) + 1| \geq \eta) &\leq \int_{-M}^M \int_{-M}^M \nu_{(k_+-2, k_++2)}(du_-, du_+) \\ &\times \mu_{\varepsilon, (x_{k_+-2}, x_{k_++2})}^{u_-, u_+} \left(\{u : |u(x_{k_+ \pm 2})| \leq M, \right. \\ &\left. u(x) \geq -1 + \gamma \text{ for all } x \in [x_{k_+-1}, x_{k_++1}], |u(x_{k_+}) - 1| \geq \eta\}, \right) \end{aligned} \quad (4.49)$$

where $\nu_{(k_+-2, k_++2)}$ represents the marginal distribution of the pair $(u(k_+ - 2), u(k_+ + 2))$.

Now we look for an upper bound for the probability inside the integral above. To do so, for $u(x_{k_+ \pm 2}) = u_{\pm}$ with $|u_{\pm}| \leq M$, we define the events $\mathcal{A}_{k_+}^{u_-, u_+}$ and $\mathcal{B}_{k_+}^{u_-, u_+}$, both only depending on the segments of a path u in the neighbourhood of x_+ :

$$\begin{aligned}\mathcal{A}_{k_+}^{u_-, u_+} &:= \{u : |u(x_{k_+ - 2})| \leq M, |u(x_{k_+ + 2})| \leq M, \\ &\quad u(x) \geq -1 + \gamma \text{ when } x \in [x_{k_+ - 1}, x_{k_+ + 1}], \quad |u(x_{k_+}) - 1| \geq \eta\}, \\ \mathcal{B}_{k_+}^{u_-, u_+} &:= B(\mathcal{A}_{k_+}^{u_-, u_+}, \gamma/2) = \{u : |u(x_{k_+ - 2})| \leq M + \gamma/2, |u(x_{k_+ + 2})| \leq M + \gamma/2, \\ &\quad u(x) \geq -1 + \gamma/2 \text{ when } x \in [x_{k_+ - 1}, x_{k_+ + 1}], \quad |u(x_{k_+}) - 1| \geq \eta - \gamma/2\}.\end{aligned}$$

Then it follows from the uniform large deviation upper bound in Lemma 4.5.6 that for any γ' small enough, there exists ε_0 such that when $\varepsilon < \varepsilon_0$,

$$\mu_{\varepsilon}(\mathcal{A}_{k_+}^{u_-, u_+}) \leq \exp\left(-\frac{1}{\varepsilon}(\Delta E(\mathcal{B}_{k_+}^{u_-, u_+})) + \gamma'\right). \quad (4.50)$$

Finally, by applying Lemma 4.5.12 to bounding the energy difference above, we see that the desired bound (4.47) follows from (4.49) and (4.50), after relabelling the small constants in the exponential. Moreover, when η is small, the constant $C(\eta)$ in (4.47) has the same order of smallness as c_{η} defined in (4.51) and is like $\mathcal{O}(\eta^2)$. Therefore after relabelling the small variable η the estimate (4.44) follows from the two steps above. \square

Lemma 4.5.12. *There exists $C < \infty$ such that for any M sufficiently large and $\gamma > 0$ small enough, there exists ℓ_* satisfying the following property. Consider u defined on $(-2\ell, 2\ell)$ with $\ell \geq \ell_*$ and boundary conditions $u_{\pm} \in [-M, M]$. Define sets*

$$\begin{aligned}\mathcal{A} &:= \{u : u(\pm 2\ell) = u_{\pm}, u \geq -1 + 2\gamma \text{ on } [-\ell, \ell]\}, \\ \tilde{\mathcal{A}} &:= \{u : u(\pm 2\ell) = u_{\pm}, u \geq -1 + \gamma/2 \text{ on } [-\ell, \ell], |u(0) - 1| \geq \eta - \gamma/2\}.\end{aligned}$$

Then it holds that

$$\inf_{u \in \tilde{\mathcal{A}}} E_{(-2\ell, 2\ell)}(u) - \inf_{u \in \mathcal{A}} E_{(-2\ell, 2\ell)}(u) \geq c_{\eta} - C\gamma,$$

where

$$c_{\eta} := 2 \min \left\{ \int_{1-\eta}^1 \sqrt{2V(u)} du, \int_1^{1+\eta} \sqrt{2V(u)} du \right\}. \quad (4.51)$$

Proof. We follow the same lines as in the proof of [180, Lemma 6.6]. First we look for a lower bound for $\inf_{u \in \tilde{\mathcal{A}}} E_{(-2\ell, 2\ell)}(u)$. In fact, for $u \in \tilde{\mathcal{A}}$, either there exists $x_1 \in (-\ell, 0)$

and $x_2 \in (0, \ell)$ such that

$$|u(x_i) - 1| \leq \gamma/2, \quad i = 1, 2,$$

or $|u(x) - 1| > \gamma/2$ on an interval of length larger than ℓ . In the latter case, one has

$$E_{(-2\ell, 2\ell)}(u) \gtrsim \ell\gamma^2. \quad (4.52)$$

In the former case, we may assume that $u(x_1) = u(x_2) = 1 - \gamma$ and $u(0) = 1 - \eta$. We can apply the Modica-Mortola trick to build a profile u connecting the following pairs: (a) u_- and $u(x_1)$, (b) $u(x_1)$ and $u(0)$, (c) $u(0)$ and $u(x_2)$, (d) $u(x_2)$ and u_+ . Moreover, it is not hard to see that

$$\inf_{u \in \tilde{\mathcal{A}}} E_{(-2\ell, 2\ell)}(u) \geq \varphi_1(u_-) + \varphi_1(u_+) + c_\eta - C\gamma. \quad (4.53)$$

Since the right side of (4.52) is larger than the right side of (4.53) for ℓ large enough, the bound (4.53) is the effective lower bound we need.

On the other hand, for $u \in \mathcal{A}$, the minimum of the energy is bounded from above by the energy over some test function u satisfying $u(\pm 2\ell) = u_\pm$ and $u(0) = 1$. As a result,

$$\inf_{u \in \mathcal{A}} E_{(-2\ell, 2\ell)}(u) \leq \varphi_1(u_-) + \varphi_1(u_+) + o(1)_{\ell \rightarrow \infty}.$$

When ℓ is large enough one has

$$\inf_{u \in \mathcal{A}} E_{(-2\ell, 2\ell)}(u) \leq \varphi_1(u_-) + \varphi_1(u_+) + \gamma. \quad (4.54)$$

Therefore the lemma is proved by combining (4.53) with (4.54). \square

Now we move forward to proving an upper bound for the integral in (4.38). For doing this, we need to introduce some more notations. Given a partition $\{x_k\}$, $k = -N_\varepsilon + 1, \dots, N_\varepsilon - 1$ of $[-\varepsilon^{-1}, \varepsilon^{-1}]$, we naturally obtain a partition $\{\tilde{x}_k\}$ of $[-1, 1]$ by defining $\tilde{x}_k = \varepsilon x_k$ and then we set $\tilde{I}_k = [\tilde{x}_{k-1}, \tilde{x}_{k+1}]$. Likewise, given an interval $\tilde{Y} \subset (-1, 1)$, we denote by \tilde{x}_{k_1} and \tilde{x}_{k_2} two endpoints to the left and to the right of \tilde{Y} respectively with distance at most $\varepsilon\ell$ from \tilde{Y} . Furthermore, one can define similar sets of paths on $(-1, 1)$ as (4.41), which will be denoted by $\tilde{\mathcal{A}}_1, \tilde{\mathcal{J}}_{\tilde{Y}}, \tilde{\mathcal{J}}_{\tilde{Y},3}^-, \tilde{\mathcal{J}}_{\tilde{Y},3}^+, \tilde{\mathcal{J}}_{\tilde{Y},3}$ respectively.

Theorem 4.5.13. *There exists $\delta_0 > 0$ such that for every $\delta \leq \delta_0$ the following holds: there exist constants $C(\delta) > 0$ and $\varepsilon_0 > 0$ such that $C(\delta) \sim \mathcal{O}(\delta^2)$ and that when $\varepsilon \leq \varepsilon_0$, we have*

$$\int_{\mathcal{A}^\delta} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \exp\left(-\frac{C(\delta)}{\varepsilon}\right). \quad (4.55)$$

Proof. With small ε and large ℓ , define $\tilde{Y} = (x_- - 4\varepsilon\ell, x_+ + 4\varepsilon\ell)$ and $Y = (x_-/\varepsilon - 4\ell, x_+/\varepsilon + 4\ell)$. We also define

$$\begin{aligned}\tilde{Y}_- &= (-1, x_- - 2\varepsilon\ell), & \tilde{Y}_+ &= (x_+ + 2\varepsilon\ell, 1), \\ Y_- &= (-1/\varepsilon, x_-/\varepsilon - 2\ell), & Y_+ &= (x_+/\varepsilon + 2\ell, 1/\varepsilon).\end{aligned}$$

We decompose all continuous paths on $[-1, 1]$ with Dirichlet boundary conditions $u(\pm 1) = \pm 1$ into the union of $\tilde{\mathcal{A}}_1$ and the following sets:

$$\begin{aligned}\mathcal{K}_{\tilde{Y}} &:= \{u \in \tilde{\mathcal{A}}_1^c : u \text{ has exactly one } \gamma^- \text{ up transition layer } \leq 2\varepsilon\ell \text{ on } \tilde{Y}\}, \\ \mathcal{K}_{\tilde{Y}_-} &:= \{u \in \tilde{\mathcal{A}}_1^c : u \text{ has exactly one } \gamma^- \text{ up transition layer } \leq 2\varepsilon\ell \text{ on } \tilde{Y}_-\}, \\ \mathcal{K}_{\tilde{Y}_+} &:= \{u \in \tilde{\mathcal{A}}_1^c : u \text{ has exactly one } \gamma^- \text{ up transition layer } \leq 2\varepsilon\ell \text{ on } \tilde{Y}_+\}, \\ \mathcal{K}_3 &:= \{u \in \tilde{\mathcal{A}}_1^c : u \text{ has one long } \gamma^- \text{ up transition layer or} \\ &\quad \text{more than one } \gamma^- \text{ up transition layer on } (-1, 1)\}.\end{aligned} \quad (4.56)$$

It is obvious that

$$\begin{aligned}\int_{\mathcal{A}^\delta} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) &\leq \int_{\mathcal{A}^\delta \cap \tilde{\mathcal{A}}_1} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \\ &+ \int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}_-}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) + \int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \\ &+ \int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}_+}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) + \int_{\mathcal{A}^\delta \cap \mathcal{K}_3} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du).\end{aligned} \quad (4.57)$$

By Lemma 4.5.8, the first term on the right can be bounded as follows

$$\int_{\mathcal{A}^\delta \cap \tilde{\mathcal{A}}_1} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \tilde{\mu}_\varepsilon(\mathcal{A}^\delta \cap \tilde{\mathcal{A}}_1) \leq \mu_\varepsilon(\mathcal{A}_1) \leq \exp\left(-\frac{M}{\varepsilon C}\right) \quad (4.58)$$

with some large $M > 0$ and $C > 0$. Moreover, it follows from Theorem 4.5.3 and Lemma 4.5.9 that

$$\begin{aligned}\int_{\mathcal{A}^\delta \cap \mathcal{K}_3} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \\ \leq \mu_\varepsilon(u \text{ has one long transition layer or three } \gamma^- \text{ up transition layers}) \\ \lesssim \exp\left(-\frac{3c_0 - \eta}{\varepsilon}\right) + \exp\left(-\frac{\ell\gamma^2}{\varepsilon}\right) \lesssim \exp\left(-\frac{3c_0 - \eta}{\varepsilon}\right)\end{aligned} \quad (4.59)$$

with $\eta > 0$ being a constant sufficiently small. The last inequality follows since the second term on the right of above is of higher order smallness when ℓ large enough. Now we find

an upper bound for the second term on the right hand side of (4.57). By the definition of the sets in (4.56), one sees that $\mathcal{J}_{Y_-} \setminus \mathcal{J}_{Y_-,3} = T_\varepsilon(K_{\tilde{Y}_-})$. Then from the definition of Φ_ε given by (4.33), we have

$$\begin{aligned}
& \int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}_-}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \int_{\mathcal{K}_{\tilde{Y}_-}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \\
& = \int_{\mathcal{J}_{Y_-} \setminus \mathcal{J}_{Y_-,3}} \exp\left(-\frac{1}{\varepsilon}\Phi_\varepsilon(u)\right) \mu_\varepsilon(du) \\
& = \int_{(\mathcal{J}_{Y_-} \setminus \mathcal{J}_{Y_-,3}) \cap \{u: |u(x_{k_-})+1| \geq 1/2\}} \exp\left(-\frac{1}{\varepsilon}\Phi_\varepsilon(u)\right) \mu_\varepsilon(du) \\
& + \int_{(\mathcal{J}_{Y_-} \setminus \mathcal{J}_{Y_-,3}) \cap \{u: |u(x_{k_-})+1| \leq 1/2\}} \exp\left(-\frac{1}{\varepsilon}\Phi_\varepsilon(u)\right) \mu_\varepsilon(du) \\
& \leq \exp\left(-\frac{\lambda}{4\varepsilon}\right) + \mu_\varepsilon((\mathcal{J}_{Y_-} \setminus \mathcal{J}_{Y_-,3}) \cap \{u: |u(x_{k_-})+1| \leq 1/2\}).
\end{aligned} \tag{4.60}$$

Additionally, using the same techniques in the proof of (4.47) we can bound the second term on the right hand side of above as

$$\mu_\varepsilon((\mathcal{J}_{Y_-} \setminus \mathcal{J}_{Y_-,3}) \cap \{u: |u(x_{k_-})+1| \leq 1/2\}) \leq \exp\left(-\frac{\varphi_1(-1/2)-\eta}{\varepsilon}\right)$$

for a small $\eta > 0$. This implies that

$$\int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}_-}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \exp\left(-\frac{\lambda}{4\varepsilon}\right) + \exp\left(-\frac{\varphi_1(-1/2)-\eta}{\varepsilon}\right).$$

The fourth term on the right side of (4.57) can be bound in the same manner, namely

$$\int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}_+}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \exp\left(-\frac{\lambda}{4\varepsilon}\right) + \exp\left(-\frac{\varphi_{-1}(1/2)-\eta}{\varepsilon}\right).$$

It remains to bound the third term on the right side of (4.57), for which we claim that there exists $C(\delta) > 0$ such that $C(\delta) \sim \mathcal{O}(\delta^2)$ and that

$$\int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \exp\left(-\frac{C(\delta)}{\varepsilon}\right). \tag{4.61}$$

Indeed, the set $\mathcal{K}_{\tilde{Y}}$ can be written in the form

$$\mathcal{K}_{\tilde{Y}} = \bigcup_{k=k_- - 4}^{k_+ + 4} \mathcal{K}_{\tilde{I}_k} := \bigcup_{k=k_- - 4}^{k_+ + 4} \{u \in \tilde{\mathcal{A}}_1^c : u \text{ has exactly one } \gamma^- \text{ transition layer on } \tilde{I}_k\}.$$

Consequently,

$$\int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{I}_k}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \sum_{k=k_-+4}^{k_++4} \tilde{\mu}_\varepsilon\left(\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{I}_k}\right). \quad (4.62)$$

For any fixed k , we denote by ξ_k the middle point of the interval \tilde{I}_k . Then from the definition of \mathcal{A}_δ , it is easy to see the following inclusion

$$\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{I}_k} \subset \{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^2(-1,1)} \geq \delta\}, \quad (4.63)$$

where $m_{\xi_k} \in \mathcal{M}_+^+$ with \mathcal{M}_+^+ defined by (4.29). Furthermore, we define the index set $\mathcal{I}_k := \{j \in -N_\varepsilon, \dots, N_\varepsilon : |j - k'| \leq 4 \text{ with } k' \in \{k, k_-, k_+\}\}$. Then using the inequality $\|u\|_{L^2(a,b)} \leq \sqrt{b-a}\|u\|_{L^\infty(a,b)}$ we have the inclusion

$$\begin{aligned} \left\{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^2(-1,1)} \geq \delta\right\} &\subset \bigcup_{j \in \mathcal{I}_k} \left\{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^2(\tilde{I}_j)} \geq \delta/48\right\} \bigcup \\ &\bigcup_{j \notin \mathcal{I}_k} \left\{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^\infty(\tilde{I}_j)} \geq \frac{\delta}{2\sqrt{2}}\right\}. \end{aligned} \quad (4.64)$$

For any $j \in \mathcal{I}_k$, we claim that there exists a constant $C > 0$ such that when $\varepsilon \ll 1$ it holds that

$$\tilde{\mu}_\varepsilon\left(\left\{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^2(\tilde{I}_j)} \geq \delta/48\right\}\right) \leq \exp\left(-\frac{C}{\varepsilon^{3/2}}\right). \quad (4.65)$$

In fact, noticing from the fact that $\|m_{\xi_k}\|_{L^\infty} = 1$, one can obtain from the same elementary norm inequality above that

$$\begin{aligned} &\tilde{\mu}_\varepsilon\left(\left\{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^2(\tilde{I}_j)} \geq \delta/48\right\}\right) \\ &\leq \tilde{\mu}_\varepsilon\left(\left\{u \in \mathcal{K}_{\tilde{I}_k} : \|u\|_{L^\infty(\tilde{I}_j)} \geq \frac{\delta}{48\sqrt{2\varepsilon\ell}} - 1\right\}\right) \\ &= \mu_\varepsilon\left(\left\{u \in \mathcal{K}_{I_k} : \|u\|_{L^\infty(I_j)} \geq \frac{\delta}{48\sqrt{2\varepsilon\ell}} - 1\right\}\right). \end{aligned} \quad (4.66)$$

Next, by the definition of the set \mathcal{K}_{I_k} (see (4.56)), we know that any path in \mathcal{K}_{I_k} takes values

in $[-M, M]$ at the nodes $\{x_k\}$. As a consequence, we have that

$$\begin{aligned}
& \mu_\varepsilon \left(\left\{ u \in \mathcal{K}_{I_k} : \|u\|_{L^\infty(I_j)} \geq \frac{\delta}{48\sqrt{2\varepsilon\ell}} - 1 \right\} \right) \\
& \leq \mu_\varepsilon \left\{ |u(x_{j\pm 1})| \leq M : \text{there exists } x_j^* \in I_j \text{ such that } |u(x_j^*)| \geq \frac{\delta}{48\sqrt{2\varepsilon\ell}} - 1 \right\} \\
& \leq \int_{-M}^M \int_{-M}^M \nu_{(j-1, j+1)}(du_-, du_+) \\
& \quad \times \mu_{\varepsilon, (x_{j-1}, x_{j+1})}^{u_-, u_+} \left(\left\{ u : \text{there exists } x_j^* \in I_j \text{ such that } |u(x_j^*)| \geq \frac{\delta}{48\sqrt{2\varepsilon\ell}} - 1 \right\} \right)
\end{aligned} \tag{4.67}$$

where as before $\nu_{(j-1, j+1)}(du_-, du_+)$ denotes the marginal distribution of the pair $(u(x_{j-1}), u(x_{j+1}))$. Moreover, according to Lemma 4.5.6, for all $|u_\pm| \leq M$, the probability inside the above integral can be bounded as follows when $\varepsilon \ll 1$:

$$\begin{aligned}
& \mu_{\varepsilon, (x_{j-1}, x_{j+1})}^{u_-, u_+} \left(\left\{ u : \text{there exists } x_j^* \in I_j \text{ such that } |u(x_j^*)| \geq \frac{\delta}{48\sqrt{2\varepsilon\ell}} - 1 \right\} \right) \\
& \leq \exp \left(-\frac{1}{\varepsilon} (\Delta E(\mathcal{B}) - 1) \right)
\end{aligned}$$

where the energy difference ΔE is defined by (4.36) and the event \mathcal{B} is given by

$$\mathcal{B} := \left\{ u(x_{j\pm 1}) = u_\pm : \text{there exists } x_j^* \in I_j \text{ such that } |u(x_j^*)| \geq \frac{\delta}{48\sqrt{2\varepsilon\ell}} - 2 \right\}.$$

Then by using the Mordica-Motola trick and taking into account of the boundary constraint $|u(x_{j\pm 1})| = |u_\pm| \leq M$, we can obtain the following bound for the energy difference: there exists $C > 0$ such that when $\varepsilon \ll 1$,

$$\begin{aligned}
\Delta(E(\mathcal{B})) & \geq \inf_{u \in \mathcal{B}} E_{(x_{j-1}, x_{j+1})}(u) - \inf_{u \in \mathcal{B}^{bc}} E_{(x_{j-1}, x_{j+1})}(u) \\
& \geq \int_M^{\delta/(48\sqrt{2\varepsilon\ell})-2} \sqrt{2V(u)} du - C_M \\
& \geq \frac{C}{\varepsilon^{3/2}}.
\end{aligned}$$

Note that in the second line above the constant C_M denotes an upper bound for the infimum $\inf_{u \in \mathcal{B}^{bc}} E_{(x_{j-1}, x_{j+1})}(u)$, which can be obtained for example by choosing u to be the linear interpolation

$$\bar{u}(x) = \frac{x - x_{j-1}}{x_{j+1} - x_{j-1}} u_+ + \frac{x_{j+1} - x}{x_{j+1} - x_{j-1}} u_-.$$

We also used that $V(u) = \frac{1}{4}(1 - u^2)^2$ in the last inequality. Therefore combining the

estimates above leads to (4.65).

In the case that $j \notin \mathcal{I}_k$ we claim that there exists $C(\delta) > 0$ such that

$$\tilde{\mu}_\varepsilon \left(\left\{ u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^\infty(\tilde{I}_j)} \geq \frac{\delta}{2\sqrt{2}} \right\} \right) \leq \exp \left(-\frac{C(\delta)}{\varepsilon} \right) \quad (4.68)$$

for ε small enough. We only prove the bound (4.68) for $j \notin \mathcal{I}_k$ and $j > k$ as the other case can be treated analogously. Noting that $m_{\xi_k} = 1$ on I_j when $j > k$, and from the definition of \mathcal{K}_Y and \mathcal{J}_Y we have

$$\begin{aligned} & \tilde{\mu}_\varepsilon \left(\left\{ u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^\infty(\tilde{I}_j)} \geq \frac{\delta}{2\sqrt{2}} \right\} \right) \\ &= \mu_\varepsilon \left(\left\{ u \in \mathcal{J}_{I_k} \setminus \mathcal{J}_{I_k,3} : \|u - 1\|_{L^\infty(I_j)} \geq \frac{\delta}{2\sqrt{2}} \right\} \right) \\ &= \mu_\varepsilon \left(\left\{ u \in \mathcal{J}_{I_k} \setminus \mathcal{J}_{I_k,3} : \exists x_j^* \in I_j \text{ such that } |u(x_j^*) - 1| \geq \frac{\delta}{2\sqrt{2}} \right\} \right). \end{aligned} \quad (4.69)$$

In addition, by using the same arguments used to obtain (4.47), we can conclude that

$$\mu_\varepsilon \left(\left\{ u \in \mathcal{J}_{I_k} \setminus \mathcal{J}_{I_k,3} : \exists x_j^* \in I_j \text{ such that } |u(x_j^*) - 1| \geq \frac{\delta}{2\sqrt{2}} \right\} \right) \leq \exp \left(-\frac{C(\delta)}{\varepsilon} \right) \quad (4.70)$$

for some $C(\delta) \sim \mathcal{O}(\delta^2)$. This proves (4.68). Consequently the bound (4.61) follows from (4.62)-(4.64), (4.65), (4.68) and the fact that $|N_\varepsilon| \lesssim \frac{1}{\varepsilon}$. In view of the established estimates for each term on the right side of (4.57), there exists $\delta_0 > 0$ such that for every $\delta \leq \delta_0$ the third term on the right side of (4.57) dominates the rest since $C(\delta) \sim \mathcal{O}(\delta^2)$. The proof is now complete. \square

4.5.3 Proof of Theorem 4.4.2

In this section we consider the data given as in Case (II), i.e. $f_\pm = \mp 1$. Remember that in this case the data-fidelity is

$$\Phi(u) = \lambda((u(x_-) - 1)^2 + (u(x_+) + 1)^2).$$

We aim to prove that the measure $\tilde{\nu}^\varepsilon$ is concentrated around the set \mathcal{M}_λ defined by (4.31).

Similar to what we did in last section, we redefine the event of interest

$$\mathcal{A}^\delta := \{u : \text{dist}_{L^2(-1,1)}(u, \mathcal{M}_\lambda) \geq \delta\}. \quad (4.71)$$

Then the probability of this event is

$$\tilde{\nu}_\varepsilon(\mathcal{A}^\delta) = \frac{1}{Z_\varepsilon} \int_{\mathcal{A}^\delta} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du). \quad (4.72)$$

with

$$Z_\varepsilon = \int \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du). \quad (4.73)$$

We prove Theorem 4.4.2 by showing a lower bound on the normalisation constant Z_ε (cf. Theorem 4.5.14) and an upper bound on the above integral (cf. Theorem 4.5.16).

We first seek a lower bound for Z_ε . As before, assume that we have the same partition $\{x_k\}$ on $(-\varepsilon^{-1}, \varepsilon^{-1})$ (cf. (4.40)) and $\{\tilde{x}_k\}$ on $(-1, 1)$ with $\tilde{x}_k = \varepsilon x_k$. The main idea for obtaining a lower bound on Z_ε is to restrict the integral (4.73) over a set of paths which almost attain the lowest energy cost. For any $\lambda > 0$, recall that ρ_λ is the lowest energy cost defined in Lemma 4.3.3.

Theorem 4.5.14. *For any small $\eta > 0$, there exists $\varepsilon_0 > 0$ such that for $\varepsilon \leq \varepsilon_0$,*

$$Z_\varepsilon \gtrsim \exp\left(-\frac{\rho_\lambda + \eta}{\varepsilon}\right). \quad (4.74)$$

Proof. Let $Y = (-1/(2\varepsilon), x_-/(2\varepsilon))$ and define sets as in (4.41). For $h > 0$, small $\eta > 0$, large $M > 0$ and sufficiently small $\gamma > 0$, by restricting the integral over the paths passing the neighbourhood of 1 and $1 - h$ at x_{k_-} and x_{k_+} respectively, we have from the definition of Φ that

$$\begin{aligned} Z_\varepsilon &= \int \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \\ &= \int \exp\left(-\frac{1}{\varepsilon}\Phi_\varepsilon(u)\right) \mu_\varepsilon(du) \\ &\geq \exp\left(-\frac{\lambda(\eta^2 + (2 - h + \gamma)^2)}{\varepsilon}\right) \\ &\quad \times \mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_-}) - 1| \leq \eta \text{ and } |u(x_{k_+}) - (1 - h)| \leq \gamma). \end{aligned} \quad (4.75)$$

We claim that there exist a constant $C > 0$ such that for sufficiently small $\gamma' > 0$ there exists $\varepsilon_0 > 0$ such that when $\varepsilon, \varepsilon_0$

$$\begin{aligned} &\mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_-}) - 1| \leq \eta \text{ and } |u(x_{k_+}) - (1 - h)| \leq \gamma) \\ &\geq C \exp\left(-\frac{c_h + \gamma'}{\varepsilon}\right), \end{aligned} \quad (4.76)$$

where c_h defined by (4.51). This would directly imply the desired estimate (4.74). In fact, combining (4.76) together with (4.75) yields

$$\begin{aligned} Z_\varepsilon &\geq C \exp \left(-\frac{(\lambda\eta^2 + \lambda(2-h)^2 + c_h) + \mathcal{O}(\gamma + \gamma')}{\varepsilon} \right) \\ &= C \exp \left(-\frac{\rho(h) + \lambda\eta^2 + \mathcal{O}(\gamma + \gamma')}{\varepsilon} \right) \\ &\gtrsim \exp \left(-\frac{\rho\lambda + \eta}{\varepsilon} \right), \end{aligned} \tag{4.77}$$

where ρ is defined in (4.15) and the last inequality follows by choosing $h = h^* := \arg \min_h \rho(h)$ and by relabelling the small quantity $(\lambda\eta^2 + \mathcal{O}(\gamma + \gamma'))$ with η .

Now we prove (4.76). First one can argue analogously to **Step 1** in the proof of Theorem 4.5.11 to obtain that when $\varepsilon \ll 1$,

$$\mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3}) \geq \frac{x_- + 1}{8}. \tag{4.78}$$

Next we can write

$$\begin{aligned} \mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_-}) - 1| \leq \eta \text{ and } |u(x_{k_+}) - (1-h)| \leq \gamma) = \\ \mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_+}) - (1-h)| \leq \gamma) - \\ \mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_-}) - 1| \geq \eta \text{ and } |u(x_{k_+}) - (1-h)| \leq \gamma). \end{aligned} \tag{4.79}$$

We now bound the two terms on the right side of above individually. In fact, by using the same arguments used to prove (4.47), we can bound the second term as follows: there exists $C(\eta) > 0$ such that

$$\begin{aligned} \mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_-}) - 1| \geq \eta \text{ and } |u(x_{k_+}) - (1-h)| \leq \gamma) \\ \leq \exp \left(-\frac{C(\eta) + c_h + \gamma'}{\varepsilon} \right). \end{aligned} \tag{4.80}$$

For the first term, we claim that for any sufficiently small $\gamma' > 0$,

$$\mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_+}) - (1-h)| \leq \gamma) \geq \exp \left(-\frac{c_h + \gamma'}{\varepsilon} \right) \mu_\varepsilon(\mathcal{J}_Y \setminus \mathcal{J}_{Y,3}). \tag{4.81}$$

Assuming the validity of above bound, the (4.76) follows directly from (4.78) since

$$\begin{aligned}
& \mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_-}) - 1| \leq \eta \text{ and } |u(x_{k_+}) - (1-h)| \leq \gamma) \\
& \geq \frac{x_- + 1}{8} \exp\left(-\frac{c_h + \gamma'}{\varepsilon}\right) - \exp\left(-\frac{C(\eta) + c_h + \gamma'}{\varepsilon}\right) \\
& \geq \frac{x_- + 1}{16} \exp\left(-\frac{c_h + \gamma'}{\varepsilon}\right)
\end{aligned} \tag{4.82}$$

when $\varepsilon \ll 1$.

Now it remains to prove (4.81). For this we need to exploit the double-sided strong Markov property of the measure μ_ε stated in Lemma 4.5.7. To be more specific, we first define the following sets

$$\begin{aligned}
\mathcal{A}_{k_1}^\ominus &:= \{u : |u(x_j)| \leq M \text{ for } j \leq k_1 - 1, u \leq (1-\gamma) \text{ on } [-1/\varepsilon, x_{k_1-1}]\}, \\
\mathcal{A}_{k_+}^\ominus &:= \{u : |u(x_j)| \leq M \text{ for } k_1 - 1 \leq j \leq k_+ - 2, \\
& u \text{ has one } \gamma^- \text{ up transition layer of length } 2\ell \text{ in } Y, u \geq (-1+\gamma) \text{ on } [x_{k_2+1}, x_{k_+-2}]\}, \\
\mathcal{A}_{k_+}^\oplus &:= \{u : |u(x_j)| \leq M \text{ for } j \geq k_+ + 2, u \geq (-1+\gamma) \text{ on } [x_{k_++2}, 1/\varepsilon]\}, \\
\mathcal{A}_{k_+}^\odot &:= \{u : |u(x_j)| \leq M \text{ for } k_+ - 2 \leq j \leq k_+ + 2, u \geq -1 + \gamma \text{ on } [x_{k_+-2}, x_{k_++2}]\}, \\
\mathcal{A}_{h,k_+}^\odot &:= \{u \in \mathcal{A}_{k_+}^\odot : |u(x_{k_+}) - (1-h)| \geq \gamma\}.
\end{aligned} \tag{4.83}$$

Then by definition, we have

$$\begin{aligned}
\{u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_+}) - (1-h)| \leq \gamma\} &= \mathcal{A}_{k_1}^\ominus \cap \mathcal{A}_{k_+}^\oplus \cap \mathcal{A}_{k_+}^\ominus \cap \mathcal{A}_{h,k_+}^\odot, \\
\mathcal{J}_Y \setminus \mathcal{J}_{Y,3} &= \mathcal{A}_{k_1}^\ominus \cap \mathcal{A}_{k_+}^\oplus \cap \mathcal{A}_{k_+}^\ominus \cap \mathcal{A}_{k_+}^\odot.
\end{aligned}$$

Furthermore, it follows from the strong Markov property that

$$\begin{aligned}
& \mu_\varepsilon(u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k_+}) - (1-h)| \leq \gamma) = \mu_\varepsilon(\mathcal{A}_{k_1}^\ominus \cap \mathcal{A}_{k_+}^\oplus \cap \mathcal{A}_{k_+}^\ominus \cap \mathcal{A}_{h,k_+}^\odot) \\
& = \frac{\mu_\varepsilon(\mathcal{A}_{k_1}^\ominus \cap \mathcal{A}_{k_+}^\oplus \cap \mathcal{A}_{k_+}^\ominus \cap \mathcal{A}_{h,k_+}^\odot)}{\mu_\varepsilon(\mathcal{A}_{k_1}^\ominus \cap \mathcal{A}_{k_+}^\oplus \cap \mathcal{A}_{k_+}^\ominus \cap \mathcal{A}_{k_+}^\odot)} \cdot \mu_\varepsilon(\mathcal{A}_{k_1}^\ominus \cap \mathcal{A}_{k_+}^\oplus \cap \mathcal{A}_{k_+}^\ominus \cap \mathcal{A}_{h,k_+}^\odot) \\
& \geq \inf_{u_-, u_+ \in [-M, M]} \frac{\mathbb{E}_{(x_{k_+-2}, x_{k_++2})}^{\mu_\varepsilon, u_-, u_+}(\mathbf{1}_{\mathcal{A}_{h,k_+}^\odot}(u))}{\mathbb{E}_{(x_{k_+-2}, x_{k_++2})}^{\mu_\varepsilon, u_-, u_+}(\mathbf{1}_{\mathcal{A}_{k_+}^\odot}(u))} \mu_\varepsilon(\mathcal{J}_Y \setminus \mathcal{J}_{Y,3}).
\end{aligned} \tag{4.84}$$

Therefore to prove (4.81) it is sufficient to show

$$\inf_{u_{\pm} \in [-M, M]} \frac{\mathbb{E}_{(x_{k_+}-2, x_{k_+}+2)}^{\mu_{\varepsilon, u_-, u_+}}(\mathbf{1}_{\mathcal{A}_{h, k_+}^{\odot}}(u))}{\mathbb{E}_{(x_{k_+}-2, x_{k_+}+2)}^{\mu_{\varepsilon, u_-, u_+}}(\mathbf{1}_{\mathcal{A}_{k_+}^{\odot}}(u))} \geq \exp\left(-\frac{c_h + \gamma'}{\varepsilon}\right). \quad (4.85)$$

On the one hand, the numerator in the above ratio can be bounded from below by using the uniform large deviation lower bound established in Lemma 4.5.5. To see this, we define the set

$$\mathcal{A} := \{u : |u(x_j)| \leq M - \gamma \text{ for } j = k_+ - 2, \dots, k_+ + 2, \\ |u(x_{k_+}) - (1 - h)| \geq 2\gamma, u \geq -1 + 2\gamma \text{ on } [x_{k_+-1}, x_{k_++1}]\}.$$

Observe that $\mathcal{A}_{h, k_+}^{\odot} = B(\mathcal{A}, \gamma)$. Then for any small $\gamma' > 0$ and for any ε small enough, we have from Lemma 4.5.5 that

$$\mu_{\varepsilon, (x_{k_+}-2, x_{k_+}+2)}^{u_-, u_+}(\mathcal{A}_{h, k_+}^{\odot}) \geq \exp\left(-\frac{1}{\varepsilon}(\Delta E(\mathcal{A}) + \gamma'/2)\right). \quad (4.86)$$

On the other hand, to obtain an upper bound for the denominator on the left side of (4.85), we apply the large deviation bound in Lemma 4.5.6. In fact, if we define

$$\tilde{\mathcal{A}} := \{u : |u(x_{k_+})| \leq M + \gamma/2, \text{ for } j = k_+ - 2, \dots, k_+ + 2, \\ u \geq -1 + \gamma/2 \text{ on } [x_{k_+-1}, x_{k_++1}]\},$$

then $\tilde{\mathcal{A}} = B(\mathcal{A}_{k_+}^{\odot}, \gamma/2)$. According to Lemma 4.5.6, it holds that

$$\mu_{\varepsilon, (x_{k_+}-2, x_{k_+}+2)}^{u_-, u_+}(\mathcal{A}_{k_+}^{\odot}) \leq \exp\left(-\frac{1}{\varepsilon}(\Delta E(\tilde{\mathcal{A}}) - \gamma'/2)\right). \quad (4.87)$$

As a consequence,

$$\frac{\mu_{\varepsilon, (x_{k_+}-2, x_{k_+}+2)}^{u_-, u_+}(\mathcal{A}_{h, k_+}^{\odot})}{\mu_{\varepsilon, (x_{k_+}-2, x_{k_+}+2)}^{u_-, u_+}(\mathcal{A}_{k_+}^{\odot})} \geq \exp\left(-\frac{1}{\varepsilon}(\inf_{u \in \mathcal{A}} E(u) - \inf_{u \in \tilde{\mathcal{A}}} E(u) + \gamma')\right). \quad (4.88)$$

Finally, (4.85) follows directly from (4.88) and Lemma 4.5.15. Hence the proof is complete. \square

Lemma 4.5.15. *There exists $C < \infty$ such that for any M sufficiently large and $\gamma > 0$ small enough, there exists ℓ_* satisfying the following property. Consider u defined on $(-2\ell, 2\ell)$*

with $\ell \geq \ell_*$ and with boundary conditions $u_{\pm} \in [-M, M]$. Define sets

$$\begin{aligned}\mathcal{A} &:= \{u : |u(x)| \leq M - \gamma \text{ for } x = -2\ell, \ell, \dots, 2\ell, |u(0) - (1 - h)| \leq 2\gamma, \\ &\quad u \geq -1 + 2\gamma \text{ on } [-\ell, \ell]\}, \\ \tilde{\mathcal{A}} &:= \{u : |u(x)| \leq M + \gamma/2 \text{ for } x = -2\ell, \ell, \dots, 2\ell, u \geq -1 + \gamma/2 \text{ on } [-\ell, \ell]\}.\end{aligned}$$

Then it holds that

$$\inf_{u \in \mathcal{A}} E_{(-2\ell, 2\ell)}(u) - \inf_{u \in \tilde{\mathcal{A}}} E_{(-2\ell, 2\ell)}(u) \leq c_h + C\gamma.$$

Proof. We first prove an upper bound for $E_{(-2\ell, 2\ell)}(u)$ for $u \in \mathcal{A}$. Let $u \in \mathcal{A}$ be such a profile satisfying the following additional properties

$$\bar{u}(\pm 2\ell) = u_{\pm}, \bar{u}(0) = 1 - h \text{ and } \bar{u}(\pm \ell) = 1 - \gamma.$$

Then it is not hard to see from the trick of Modica-Mortola that

$$\inf_{u \in \mathcal{A}} E_{(-2\ell, 2\ell)}(u) \leq E_{(-2\ell, 2\ell)}(\bar{u}) \leq \varphi_1(u_-) + \varphi_1(u_+) + c_h + C\gamma. \quad (4.89)$$

Furthermore, if $u \in \tilde{\mathcal{A}}$, then either $u \leq 1 - \gamma/2$ over an interval of length ℓ or there exist $x_1 \in (-\ell, 0)$ and $x_2 \in (0, \ell)$ such that $u(x_i) \geq 1 - \gamma/2$, $i = 1, 2$. In the former case we have

$$E_{(-2\ell, 2\ell)}(u) \geq \ell\gamma^2,$$

while in the later case

$$E_{(-2\ell, 2\ell)}(u) \geq \varphi_1(u_-) + \varphi_1(u_+) + C\gamma. \quad (4.90)$$

Therefore when ℓ is large enough we could assume that we are in the later case. Consequently, the lemma is proved by (4.89) and (4.90). \square

We continue to bound the integral in (4.72).

Theorem 4.5.16. Fix a $\lambda > 0$. There exists $\delta_0 > 0$ such that for every $\delta \leq \delta_0$ the following holds: There exist $C(\delta) > 0$ and $\varepsilon_0 > 0$ such that $C(\delta) \sim \mathcal{O}(\delta^2)$ and that for $\varepsilon \leq \varepsilon_0$ we have

$$\int_{\mathcal{A}^\delta} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \exp\left(-\frac{C(\delta) + \rho_\lambda}{\varepsilon}\right). \quad (4.91)$$

Proof. We only consider the case where $0 < \lambda < 2$ since the other cases can be treated

in the same way (see Remark 4.5.17). The idea of the proof is similar to that of Theorem 4.5.13. For $\ell > 0$ and $\varepsilon > 0$, we define the following intervals

$$\begin{aligned}\tilde{Y}_- &= (-1, x_- - 4\varepsilon\ell), \tilde{Y}_+ = (x_+ + 4\varepsilon\ell, 1), \tilde{Y} = (x_- + 2\varepsilon\ell, x_+ - 2\varepsilon\ell) \\ Y_- &= (-1/\varepsilon, x_-/\varepsilon - 4\ell), Y_+ = (x_+/\varepsilon + 4\ell, 1/\varepsilon), Y = (x_-/\varepsilon + 2\ell, x_+/\varepsilon - 2\ell).\end{aligned}$$

One can first decompose all continuous paths on $[-1, 1]$ with Dirichlet boundary conditions $u(\pm 1) = \pm 1$ into the union of \tilde{A}_1 and the sets $\mathcal{K}_{\tilde{Y}_-}, \mathcal{K}_{\tilde{Y}}, \mathcal{K}_{\tilde{Y}_+}, \mathcal{K}_3$ defined in (4.56). Thus (4.57) still holds. Remember that $\Phi(u) = \lambda((u(x_-) - 1)^2 + (u(x_+) - 1)^2)$. For paths belonging to \tilde{A}_1 and $\tilde{\mathcal{K}}_3$, we have the same bounds as (4.58) and (4.59). In addition, if $0 < \lambda < 2$, then we claim that for small $\eta > 0$,

$$\int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \exp\left(-\frac{2\rho_\lambda - \eta}{\varepsilon}\right) \quad (4.92)$$

for ε small enough. To see this, let $\{B_r(h_j)\}_{j=1}^{N_r}$ be a collection of open balls of radius r covering $[-M, M]$ where the centres $h_j \in [-M, M]$ and $N_r = \mathcal{O}(1/r)$. Notice that $\mathcal{J}_Y \setminus \mathcal{J}_{J,3} = T_\varepsilon(\mathcal{K}_{\tilde{Y}})$, so we have

$$\begin{aligned}& \int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \\ & \leq \sum_{j=1}^{N_r} \sum_{k=1}^{N_r} \int_{\{u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k-}) - h_j| \leq r, |u(x_{k+}) - h_k| \leq r\}} \exp\left(-\frac{1}{\varepsilon}\Phi_\varepsilon(u)\right) \mu_\varepsilon(du).\end{aligned} \quad (4.93)$$

For fixed j and k , using the same trick (based on the strong Markov property) as in the proof of (4.81), one can obtain the following estimate: for any small $r > 0$, there exists $C > 0$ such that when ε small enough,

$$\begin{aligned}& \int_{\{u \in \mathcal{J}_Y \setminus \mathcal{J}_{Y,3} : |u(x_{k-}) - h_j| \leq r, |u(x_{k+}) - h_k| \leq r\}} \exp\left(-\frac{1}{\varepsilon}\Phi_\varepsilon(u)\right) \mu_\varepsilon(du) \\ & \leq \exp\left(-\frac{\rho(1 - h_j) + \rho(1 - h_k) - Cr}{\varepsilon}\right) \leq \exp\left(-\frac{2\rho_\lambda - Cr}{\varepsilon}\right).\end{aligned} \quad (4.94)$$

Here the function $\rho(\cdot)$ is defined by (4.15) and we used the fact that $\rho_\lambda = \min_h \rho(h)$ in the last inequality. Therefore, it holds that

$$\int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \lesssim \frac{1}{r^2} \exp\left(-\frac{2\rho_\lambda - Cr}{\varepsilon}\right) \leq \exp\left(-\frac{2\rho_\lambda - \eta}{\varepsilon}\right) \quad (4.95)$$

with appropriate small η such that $\eta > r > 0$. In addition, we assert that there exists

$C(\delta) > 0$ such that $C(\delta) \sim \mathcal{O}(\delta^2)$ and

$$\int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}_\pm}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \exp\left(-\frac{C(\delta) + \rho_\lambda}{\varepsilon}\right). \quad (4.96)$$

We only prove this for $\mathcal{K}_{\tilde{Y}_-}$ as the other one follows analogously. To do this, we decompose $\mathcal{K}_{\tilde{Y}_-}$ into

$$\mathcal{K}_{\tilde{Y}_-} := \bigcup_{k=-N_\varepsilon}^{k_-+4} \mathcal{K}_{\tilde{I}_k} := \bigcup_{k=-N_\varepsilon}^{k_-+4} \{u \in \tilde{\mathcal{A}}_1^c : u \text{ has exactly one } \gamma^- \text{ transition layer on } \tilde{I}_k\}.$$

It follows that

$$\int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{Y}_-}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \sum_{k=-N_\varepsilon}^{k_-+4} \int_{\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{I}_k}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du). \quad (4.97)$$

For any fixed k , the inclusion (4.63) still holds, namely

$$\mathcal{A}^\delta \cap \mathcal{K}_{\tilde{I}_k} \subset \{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^2(-1,1)} \geq \delta\},$$

where $\xi_k \in \tilde{I}_k$ and $m_{\xi_k} \in \mathcal{M}_\lambda$ with \mathcal{M}_λ defined by (4.31). Moreover, if we redefine the index set $\mathcal{I}_k := \{j \in -N_\varepsilon, \dots, N_\varepsilon : |j - k'| \leq 8 \text{ with } k' \in \{k, k_-, k_+\}\}$, then

$$\begin{aligned} \left\{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^2(-1,1)} \geq \delta\right\} &\subset \bigcup_{j \in \mathcal{I}_k} \left\{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^2(\tilde{I}_j)} \geq \delta/96\right\} \bigcup \\ &\bigcup_{j \notin \mathcal{I}_k} \left\{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^\infty(\tilde{I}_j)} \geq \frac{\delta}{2\sqrt{2}}\right\}. \end{aligned} \quad (4.98)$$

For $j \in \mathcal{I}_k$, as an analogue to (4.65) we have that when ε is small enough,

$$\begin{aligned} &\int_{\mathcal{A}^\delta \cap \left\{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^2(\tilde{I}_j)} \geq \delta/96\right\}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \\ &\leq \tilde{\mu}_\varepsilon\left(\left\{u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^2(\tilde{I}_j)} \geq \delta/96\right\}\right) \lesssim \exp\left(-\frac{1}{\varepsilon^{3/2}}\right). \end{aligned} \quad (4.99)$$

As for $j \notin \mathcal{I}_k$, one can argue in the same way as in the proof of (4.68) that for ε

small enough

$$\int_{\mathcal{A}^\delta \cap \left\{ u \in \mathcal{K}_{\tilde{I}_k} : \|u - m_{\xi_k}\|_{L^\infty(\tilde{I}_j)} \geq \frac{\delta}{2\sqrt{2}} \right\}} \exp\left(-\frac{1}{\varepsilon}\Phi(u)\right) \tilde{\mu}_\varepsilon(du) \leq \exp\left(-\frac{C(\delta) + \rho_\lambda}{\varepsilon}\right) \quad (4.100)$$

with $C(\delta) \sim \mathcal{O}(\delta^2)$. Therefore the desired estimate (4.91) follows from (4.99)-(4.100) and (4.92) since $C(\delta)$ can be chosen smaller than ρ_λ when δ is small. □

Remark 4.5.17. *In the case that $\lambda > 2$, we still have (4.91). In fact, one can first neglect the integral on the left of (4.91) over profiles with either one or more than three transition layers as it is higher order exponentially small. Then for profiles exhibiting three transition layers, the integral over the intersection of \mathcal{A}^δ and the profiles with three transition layers which fit with the data dominates the rest. Finally the result corresponding to $\lambda = 2$ follows directly from those in previous two cases.*

Chapter 5

Gaussian Approximations for Transition Paths

5.1 Introduction

Determining the behaviour of transition paths of complex molecular dynamics is essential for understanding many problems in physics, chemistry and biology. Direct simulation of these systems can be prohibitively expensive, mainly due to the fact that the dynamical systems can exhibit the phenomenon of *metastability*, which involves disparate time scales: the transition *between* metastable states is logarithmic in the inverse temperature, whilst the fluctuations *within* the metastable states have durations which are exponential in the inverse temperature. In many systems the interest is focused on the transition between metastable states and not the local fluctuations within them. This chapter addresses the problem of characterising the most likely transition paths of molecular models of chemical reactions.

We focus on the Brownian dynamics model from molecular dynamics which takes the form of a gradient flow in a potential, subject to small additive thermal noise:

$$dx(t) = -\nabla V(x(t))dt + \sqrt{2\varepsilon}dW(t); \quad (5.1)$$

we study the equation subject to the end-point conditions

$$x(0) = x_-, \quad x(T) = x_+. \quad (5.2)$$

Here $V : \mathbf{R}^d \rightarrow \mathbf{R}$ is the potential function, W is a standard Brownian motion in \mathbf{R}^d and $\varepsilon > 0$ is a small parameter related to the temperature of the thermal system. The Brownian dynamics model is widely used in the study of molecular dynamics [148]. It is also referred to as the overdamped Langevin equation, and can be derived from the second or-

der Langevin dynamics model, which has the form of damped-driven Newtonian dynamics with potential energy V , by taking a large friction or a small mass limit; see [184, Chapter 7, Exercise 8] and [148] for explicit derivations.

Mathematically we understand the process $x(t), t \in [0, T]$ satisfying (5.1), (5.2) to be the initial value problem of (5.1) starting from $x(0) = x_-$, subject to the conditioning $x(T) = x_+$ [112]. We propose to study the sample path of this conditioned process as a model for the temporal evolution of molecules making a transition between two atomistic configurations x_{\pm} . In this chapter, we will assume that x_{\pm} are critical points of V ; indeed most interest focuses on the case where both endpoints are chosen to be local minima of V .

When the temperature ε is small and when the end-point condition on $x(T)$ is removed, typical realisations of (5.1) exhibit fluctuations around the local minima of V for long stretches of time (exponential in ε^{-1}) while the occasional rapid transitions between different minima occur on a much shorter time scale which is only logarithmic in ε^{-1} . The difference between these time scales makes it difficult to sample transition paths when ε is small. As an alternative to direct sampling, several notions of “most likely transition paths” have been proposed; of particular interest here are the Freidlin-Wentzell and Onsager-Machlup theories.

In the zero temperature limit $\varepsilon \rightarrow 0$, the behaviour of transition paths can be predicted with overwhelming probability using Freidlin-Wentzell theory [98]. For any fixed T , the solution process $\{x(t), t \in [0, T]\}$ to (5.1), (5.2) satisfies a large deviation principle with rate (or action) functional given by

$$\bar{S}_T(\varphi) := \frac{1}{4} \int_0^T |\varphi'(t) + \nabla V(\varphi(t))|^2 dt \quad (5.3)$$

with $\varphi \in H_{\pm}^1(0, T; \mathbf{R}^d) := \{x \in H^1(0, T; \mathbf{R}^d) : x(0) = x_-, x(T) = x_+\}$. Loosely speaking the large deviation principle states that for any small $\delta > 0$, the probability that the solution x lies in a tube of width δ around a given path φ is approximately given by

$$\mathbb{P}\{x : \sup_{t \in [0, T]} |x(t) - \varphi(t)| \leq \delta\} \approx \exp(-\varepsilon^{-1} \bar{S}_T(\varphi)) \quad (5.4)$$

for ε small enough. Here \mathbb{P} denotes the law of the process defined in (5.1), (5.2). The large deviation principle thus characterises the exponential tail of the distribution of the transition paths; but what is of most interest to us is that it leads to a natural variational definition of the most likely path: the minimiser of the rate functional \bar{S}_T can be interpreted as most likely path in the sense that the probability of a trajectory in a small neighbourhood of this minimiser is exponentially larger in ε^{-1} than the probability of hitting neighbourhoods of any other paths.

In view of the boundary conditions (5.2), one can rewrite the functional \bar{S}_T as

$$\begin{aligned}\bar{S}_T(\varphi) &:= \frac{1}{4} \int_0^T |\varphi'(t) + \nabla V(\varphi(t))|^2 dt \\ &= \frac{1}{4} \int_0^T |\varphi'(t)|^2 + |\nabla V(\varphi(t))|^2 dt + \frac{1}{2} \int_0^T \varphi'(t) \cdot \nabla V(\varphi(t)) dt \\ &= \frac{1}{4} \int_0^T |\varphi'(t)|^2 + |\nabla V(\varphi(t))|^2 dt + \frac{1}{2} ((V(x_+) - V(x_-))).\end{aligned}\tag{5.5}$$

The last term in this expression only depends on the boundary conditions and not on the specific choice of φ . Hence minimising $\bar{S}_T(\varphi)$ is equivalent to minimising the following Freidlin-Wentzell functional

$$S_T(\varphi) := \frac{1}{4} \int_0^T |\varphi'(t)|^2 + |\nabla V(\varphi(t))|^2 dt\tag{5.6}$$

over $H_{\pm}^1(0, T; \mathbf{R}^d)$, and from now on we refer to the minimisation of this functional as the Freidlin-Wentzell approach. The Freidlin-Wentzell viewpoint has been enormously influential in the study of chemical reactions. For example the elastic band method [135] and the string method [80, 82] are numerical methods for finding minimal energy paths based on minimisation of the action functional (5.3). See the review article [220] for recent development of transition path theory.

At finite temperature $\varepsilon > 0$, optimal transition paths can be defined as minimisers of the Onsager-Machlup functional [78]. This functional is defined by maximising small ball probabilities for paths $x(\cdot)$ solving (5.1), (5.2). To be more precise, we denote by \mathbb{P}_0 the law of the Brownian bridge on $[0, T]$ connecting x_- and x_+ , corresponding to vanishing drift ($V = 0$) in (5.1), (5.2), which depends on ε . Then under certain conditions on V (see (ii) of Remark 5.2.2), the measure \mathbb{P} is absolutely continuous with respect to \mathbb{P}_0 and the Radon-Nikodym density is given by

$$\frac{d\mathbb{P}}{d\mathbb{P}_0}(x) = \frac{1}{Z} \exp\left(-\frac{1}{2\varepsilon} \int_0^T \Psi_{\varepsilon}(x(t)) dt\right)\tag{5.7}$$

where

$$\Psi_{\varepsilon}(x) := \frac{1}{2} |\nabla V(x)|^2 - \varepsilon \Delta V(x).\tag{5.8}$$

Equation (5.7) follows from Girsanov formula and Itô's formula, see [189, Section 2]. We

define the Onsager-Machlup functional I_ε over the space $H_\pm^1(0, T; \mathbf{R}^d)$ by

$$I_\varepsilon(x) := \frac{1}{2} \int_0^T \left(\frac{1}{2} |x'(t)|^2 + \Psi_\varepsilon(x(t)) \right) dt = S_T(x) - \frac{\varepsilon}{2} \int_0^T \Delta V(x(t)) dt. \quad (5.9)$$

In [78] it was shown that for any $x_1, x_2 \in H_\pm^1(0, T; \mathbf{R}^d)$

$$\lim_{\delta \rightarrow 0} \frac{\mathbb{P}(B_\delta(x_1))}{\mathbb{P}(B_\delta(x_2))} = \exp \left(\frac{1}{\varepsilon} (I_\varepsilon(x_2) - I_\varepsilon(x_1)) \right)$$

where $B_r(x)$ denotes a ball in $C([0, T]; \mathbf{R}^d)$ with centre x and radius r . Hence for any fixed x_2 , the above ratio of the small ball probability, as a function of x_1 , is maximised at minimisers of I_ε . In this sense minimisers of I_ε are analogous to *Maximum A Posterior (MAP) estimators* which arise for the posterior distribution \mathbb{P} in Bayesian inverse problems; see [63].

The Onsager-Machlup functional (5.9) differs from the Freidlin-Wentzell functional only by the integral of the Itô correction term $\varepsilon \Delta V$. This difference arises because of the order in which the limits $\varepsilon \rightarrow 0$ and $\delta \rightarrow 0$ are taken: in Freidlin-Wentzell theory the radius of the ball δ is fixed and limit $\varepsilon \rightarrow 0$ is studied while in Onsager-Machlup theory ε is fixed and limit $\delta \rightarrow 0$ is studied. For fixed $T > 0$, it is clear that $I_\varepsilon(\varphi) \rightarrow S_T(\varphi)$ as $\varepsilon \rightarrow 0$. Hence for fixed time scale T the Onsager-Machlup theory agrees with the Freidlin-Wentzell theory in the low temperature limit. However, this picture can be different for large T , more precisely when $T \rightarrow \infty$ as $\varepsilon \rightarrow 0$. In fact, as demonstrated in [188], it is possible that when $T \gg 1$, the MAP transition path spends a vast amount of time at a saddle point of V rather than at minima; moreover, for two paths with the same energy barrier, the one passing through steeper confining walls is always preferred to the other since a larger value of ΔV gives rise to a lower value of I_ε . The discussion about the order of limits gives a clue as to why this apparent contradiction occurs: by studying the limit $\delta \rightarrow 0$ in Onsager-Machlup theory, for fixed temperature ε , we remove entropic effects.

Both minimising the Onsager-Machlup functional (5.9) or finding MAP estimators are attempts to capture key properties of the distribution \mathbb{P} by identifying a single most likely path. This can be viewed as approximating the measure \mathbb{P} by a Dirac measure in a well-chosen point. The key idea in this chapter is to find better approximations to ν by working in a larger class of measures than Diracs. We will study the best Gaussian approximations with respect to Kullback-Leibler divergence. The mean of an optimal Gaussian should capture the concentration of the target measure while its fluctuation characteristics are described by the covariance of the Gaussian. Furthermore the fluctuations can capture entropic effects. Thus by using the Gaussian approximation we aim to overcome the shortcomings of the Onsager-Machlup approach. The idea of finding Gaussian approxima-

tions for non-Gaussian measures by means of the Kullback-Leibler divergence is not new. For example, in the community of machine learning [194], Gaussian processes have been widely used together with Bayesian inference for regression and prediction. Similar ideas have also been used to study models in ocean-atmosphere science [161] and computational quantum mechanics [14]. Recently, the problem of minimising the Kullback-Leibler divergence between non-Gaussian measures and certain Gaussian classes was studied from the calculus of variation point of view [187] and numerical algorithms for Kullback-Leibler minimisation were discussed in [190].

The present chapter builds on the theory developed in [187] and extends it to transition path theory. More specifically, the set of Gaussian measures for approximations is parameterised by a pair of functions (m, \mathbf{A}) , where m represents the mean and \mathbf{A} (defined in (5.18)) is used to define the covariance operator for the underlying Gaussian measure. For a fixed temperature ε , the Kullback-Leibler divergence is expressed as a functional F_ε depending on (m, \mathbf{A}) and existence of minimisers is shown in this framework. Then the asymptotic behaviour of the best Gaussian approximations in the low temperature limit is studied in terms of the Γ -convergence of the functionals $\{F_\varepsilon\}$. The limiting functional (see (5.57)) is identified as the sum of two parts. The first part, depending only on m , is identical to the Γ -limit of the rescaled Freidlin-Wentzell action functional, implying that for $\varepsilon \rightarrow 0$ the most likely transition paths defined as the best Gaussian mean m coincide with large deviation paths. The second part takes entropic effects into account and expresses the penalty for the fluctuations in terms of \mathbf{A} ; it vanishes if $\mathbf{A} = D^2V(m(t))$ but this choice of \mathbf{A} is only admissible if the Hessian $D^2V(m)$ is positive definite. A strictly positive penalty occurs when $D^2V(m(t))$ has a negative eigenvalue. Therefore minimising the limiting functional amounts to selecting those optimal paths m among the large deviation paths that do not spend time in saddles or local maximisers. We stress that although at finite noise intensity $\varepsilon > 0$ there is no explicit characterisation of our most likely transition paths, it is possible to approximately determine them numerically, as demonstrated in [190], see also Section 5.5.

This chapter is organised as follows. In the next section we introduce a time-rescaling of the governing Langevin equation, in terms of ε , in which the undesirable effects of the Onsager-Machlup minimisation are manifest; we also introduce some notation used throughout this chapter. Furthermore, assumptions on the potential V are discussed. In Section 5.3, we define the subset of Gaussian measures over which Kullback-Leibler minimisation is conducted; the existence of minimisers to the variational problem is established at the end of this section. Then in Section 5.4, we study the low temperature limit of the Gaussian approximation using Γ -convergence. The main Γ -convergence result is given in Theorem 5.4.5. Section 5.5 discusses some important consequences of the Γ -convergence

result, with emphasis on the link with theories of Freidlin-Wentzell and Onsager-Machlup. The proofs of Theorem 5.4.5 and some related results are presented in Section 5.6.

5.2 Set-up and Notation

5.2.1 Set-up

As discussed in the previous section, the key issue which motivates our work is the difference in behaviour between minimisers of the Freidlin-Wentzell action and the Onsager-Machlup functional. This difference is manifest when $T \gg 1$ and is most cleanly described by considering the time scale $T = \varepsilon^{-1}$. The Γ -limit of the Onsager-Machlup functional (5.9) is studied, as $\varepsilon \rightarrow 0$, under this time-rescaling, in [189]; the limit exhibits the undesirable effects described in the preceding section. Our objective is to characterise the Γ -limit for the variational problems arising from best Gaussian approximation with respect to the Kullback-Leibler divergence.

Applying the time scaling $t \mapsto \varepsilon^{-1}t$ to the equation (5.1) and noticing the boundary conditions (5.2), yields

$$\begin{aligned} dx(t) &= -\varepsilon^{-1} \nabla V(x(t))dt + \sqrt{2}dW(t), \\ x(0) &= x_-, \quad x(1) = x_+. \end{aligned} \tag{5.10}$$

The transformed SDE has an order one noise but a strong drift; it will be our object of study throughout the remainder of this chapter. For technical reasons, we make the following assumptions on the potential V .

Assumptions 5.2.1. *The potential V appearing in (5.10) satisfies:*

(A-1) $V \in C^5(\mathbf{R}^d)$;

(A-2) *The set of critical points*

$$\mathcal{E} := \{x \in \mathbf{R}^d, \nabla V(x) = 0\} \tag{5.11}$$

is finite and the Hessian $D^2V(x)$ is non-degenerate for any $x \in \mathcal{E}$.

(A-3) *Coercivity condition:*

$$\exists R > 0 \text{ such that } \inf_{|x| > R} |\nabla V(x)| > 0; \tag{5.12}$$

(A-4) *Growth condition:*

$$\exists C_1, C_2 > 0 \text{ and } \alpha \in [0, 2) \text{ such that for all } x \in \mathbf{R}^d \text{ and } 1 \leq i, j, k \leq d, \quad (5.13)$$

$$\limsup_{\varepsilon \rightarrow 0} \max \left(\left| \frac{\partial^3}{\partial x_i \partial x_j \partial x_k} \Psi_\varepsilon(x) \right|, |\Psi_\varepsilon(x)| \right) \leq C_1 e^{C_2 |x|^\alpha};$$

(A-5) $V(x) \rightarrow \infty$ when $|x| \rightarrow \infty$ and there exists $R > 0$ such that

$$2\Delta V(x) \leq |\nabla V(x)|^2 \text{ for } |x| \geq R; \quad (5.14)$$

(A-6) *Monotonicity condition:*

$$\exists R > 0 \text{ such that } |\nabla V(x_1)| \geq |\nabla V(x_2)| \text{ if } |x_1| \geq |x_2| \geq R. \quad (5.15)$$

Remark 5.2.2. (i) Conditions (A-2)-(A-3) are typical assumptions for proving Γ -convergence results for Ginzburg-Landau and related functionals [96, 149]. The smoothness condition (A-1) is needed because our analysis involves a Taylor expansion of order three for Ψ_ε . Furthermore, we will use conditions (A-4)-(A-6) to analyse the Γ -convergence problem in this Chapter. These assumptions will be employed to simplify the expectation term in the Kullback-Leibler divergence (see the expression (5.41)).

(ii) The condition (A-5) is a Lyapunov type condition which guarantees that at small temperature ($\varepsilon \leq 1$) the solution to the SDE in (5.10) does not explode in finite time. The probability measure determined by this process is absolutely continuous with respect to the reference measure of the Brownian bridge. See [201, Chapter 2] for more discussions about the absence of explosion. Moreover, by the definition of Ψ_ε , (A-5) implies that for any $\delta \in \mathbf{R}$ there exists a constant $C > 0$ depending only R and δ such that

$$|\nabla V(x)|^2 - \varepsilon \delta \Delta V(x) \geq -C\varepsilon \text{ for any } x \in \mathbf{R}^d. \quad (5.16)$$

Such lower bound will be used to prove the compactness of the functionals of interest (see Proposition 5.4.4).

(iii) These conditions are not independent. For instance, the coercivity condition (A-3) can be deduced from the monotonicity condition (A-6) when $V(x)$ is non-constant for large $|x|$. Hence particularly (A-5) and (A-6) imply (A-3).

(iv) The set of functions satisfying conditions (A-1)-(A-7) is not empty: they are fulfilled by all polynomials. Therefore many classical potentials, such as the Ginzburg-Landau

double-well potential $V(x) = \frac{1}{4}x^2(1-x)^2$ are included. \square

For $\varepsilon > 0$ we denote by μ_ε the law of the above bridge process x defined in (5.10) and μ_0 the law of the corresponding bridge for vanishing drift ($V = 0$) in (5.10). Then, by identical arguments to those yielding (5.7), μ_ε is absolutely continuous with respect to μ_0 and the Radon-Nikodym density is given by

$$\frac{d\mu_\varepsilon}{d\mu_0}(x) = \frac{1}{Z_{\mu,\varepsilon}} \exp\left(-\frac{1}{2\varepsilon^2} \int_0^1 \Psi_\varepsilon(x(t))dt\right) \quad (5.17)$$

where Ψ_ε is given by (5.8) and $Z_{\mu,\varepsilon}$ is the normalisation constant. Note that the extra factor $\frac{1}{\varepsilon}$ with respect to (5.7) is due to the time rescaling.

5.2.2 Notation

Throughout the chapter, we use C (or occasionally C_1 and C_2) to denote a generic positive constant which may change from one expression to the next and is independent of the temperature and any quantity of interest. We write $A \lesssim B$ if $A \leq CB$. Given an interval $I \subset \mathbf{R}$, let $L^p(I)$ and $W^{m,p}(I)$ with $m \in \mathbf{N}, 1 \leq p \leq \infty$ be the standard Lebesgue and Sobolev spaces of scalar functions respectively. Let $H^m(I) = W^{m,2}(I)$. For $s \in [0, 1]$, we set $H_0^s(I)$ to be the closure of $C_0^\infty(I)$ in $H^s(I)$ and equip it with the topology induced by $H^s(I)$. Define its dual space $H^{-s}(I) := (H_0^s(I))'$. For $s > 1/2$, a function of $H_0^s(I)$ has zero boundary conditions. Thanks to the Poincaré inequality, the H^1 -semi-norm is an equivalent norm on $H_0^1(I)$. In the case that $I = (0, 1)$, we simplify the notations by setting $H_0^s = H_0^s(0, 1)$ and $H^{-s} = H^{-s}(0, 1)$.

We write scalar and vector variables in regular face whereas matrix-valued variables, function spaces for vectors and matrices are written in boldface. Denote by $\mathcal{S}(d, \mathbf{R})$ the set of all real symmetric $d \times d$ matrices and by \mathbf{I}_d the identity matrix of size d . Let $L^p(0, 1; \mathbf{R}^d)$ and $L^p(0, 1; \mathcal{S}(d, \mathbf{R}))$ be the spaces of vector-valued and symmetric matrix-valued functions with entries in $L^p(0, 1)$ respectively. Similarly one can define $H^1(0, 1; \mathbf{R}^d)$, $H_0^s(0, 1; \mathbf{R}^d)$ and $H^1(0, 1; \mathcal{S}(d, \mathbf{R}))$. For simplicity, we use the same notation $\mathbf{L}^p(0, 1)$ (respectively $\mathbf{H}^1(0, 1)$) to denote $L^p(0, 1; \mathcal{S}(d, \mathbf{R}))$ and $L^p(0, 1; \mathbf{R}^d)$ (respectively $H^1(0, 1; \mathcal{S}(d, \mathbf{R}))$ and $H^1(0, 1; \mathbf{R}^d)$). For any $\mathbf{A} = (A_{ij}) \in L^p(0, 1; \mathcal{S}(d, \mathbf{R}))$ with $1 \leq p \leq \infty$, we define its norm

$$\|\mathbf{A}\|_{\mathbf{L}^p(0,1)} := \left(\sum_{i=1}^d \sum_{j=1}^d \|A_{ij}\|_{L^p(0,1)}^2 \right)^{\frac{1}{2}}.$$

For $\mathbf{A} = (A_{ij}) \in H^1(0, 1; \mathcal{S}(d, \mathbf{R}))$, the norm is defined by

$$\|\mathbf{A}\|_{\mathbf{H}^1(0,1)} := \left(\sum_{i=1}^d \sum_{j=1}^d \|A_{ij}\|_{H^1(0,1)}^2 \right)^{\frac{1}{2}}.$$

We also define $\mathbf{H}_{\pm}^1(0, 1) := H_{\pm}^1(0, 1; \mathbf{R}^d) := \{x \in H^1(0, 1; \mathbf{R}^d) : x(0) = x_-, x(1) = x_+\}$. Denote by $\mathbf{BV}(I)$ the set of \mathbf{R}^d -valued functions of bounded variations on an interval $I \subset \mathbf{R}$.

For matrices $\mathbf{A}, \mathbf{B} \in \mathcal{S}(d, \mathbf{R})$ we write $\mathbf{A} \geq \mathbf{B}$ when $\mathbf{A} - \mathbf{B}$ is positive semi-definite. The trace of a matrix \mathbf{A} is denoted by $\text{Tr}(\mathbf{A})$. Denote by \mathbf{A}^T the transpose of \mathbf{A} and by $|\mathbf{A}|_F$ the Frobenius norm of \mathbf{A} . Given $\mathbf{A} \in \mathcal{S}(d, \mathbf{R})$ with the diagonalised form $\mathbf{A} = \mathbf{P}^T \mathbf{\Lambda} \mathbf{P}$, we define the matrix matrix $|\mathbf{A}| := \mathbf{P}^T |\mathbf{\Lambda}| \mathbf{P}$. For matrices $\mathbf{A} = (A_{ij})$ and $\mathbf{B} = (B_{ij})$, we write

$$\mathbf{A} : \mathbf{B} = \text{Tr}(\mathbf{A} \mathbf{B}^T) = \sum_{i=1}^d \sum_{j=1}^d A_{ij} B_{ij}.$$

Define the matrix-valued operator $\partial_t^2 := \partial_t^2 \cdot \mathbf{I}_d$. For $a > 0$, we define

$$\mathbf{L}_a^1(0, 1) := L_a^1(0, 1; \mathcal{S}(d, \mathbf{R})) = \{\mathbf{A} \in L^1(0, 1; \mathcal{S}(d, \mathbf{R})) : \mathbf{A}(t) \geq a \cdot \mathbf{I}_d \text{ a.e. on } (0, 1)\}$$

and

$$\mathbf{H}_a^1(0, 1) := H_a^1(0, 1; \mathcal{S}(d, \mathbf{R})) = \{\mathbf{A} \in H^1(0, 1; \mathcal{S}(d, \mathbf{R})) : \mathbf{A}(t) \geq a \cdot \mathbf{I}_d \text{ a.e. on } (0, 1)\}.$$

We write $\mathbf{A}_n \rightharpoonup \mathbf{A}$ in $\mathbf{L}^1(0, 1)$ when \mathbf{A}_n converges to \mathbf{A} weakly in $\mathbf{L}^1(0, 1)$. Let $\mathbf{H}_0^1(0, 1) = H_0^1(0, 1; \mathbf{R}^d)$. Define $\mathbf{H}_0^s = \overbrace{H_0^s \times \cdots \times H_0^s}^d$ and let \mathbf{H}^{-s} be the dual. In addition, we define product spaces $\mathcal{H} := \mathbf{H}_{\pm}^1(0, 1) \times \mathbf{H}^1(0, 1)$, $\mathcal{H}_a := \mathbf{H}_{\pm}^1(0, 1) \times \mathbf{H}_a^1(0, 1)$, $\mathcal{X} := \mathbf{L}^1(0, 1) \times \mathbf{L}^1(0, 1)$ and $\mathcal{X}_a := \mathbf{L}^1(0, 1) \times \mathbf{L}_a^1(0, 1)$.

For a vector field $v = (v_1, v_2, \dots, v_d)$, let $\nabla v = (\partial_i v_j)_{i,j=1,2,\dots,d}$ be its gradient, which is a second order tensor (or matrix). Given a potential $V : \mathbf{R}^d \rightarrow \mathbf{R}$, denote by $D^2 V$ the Hessian of V . Given a second order tensor $\mathbf{T} = (T_{ij})_{i,j=1,2,\dots,d}$, we denote by $\nabla \mathbf{T}$ its gradient, which is a rank 3 tensor with $(\nabla \mathbf{T})_{ijk} = \frac{\partial T_{ij}}{\partial x_k}$. In particular, we use $D^3 V$ to denote the gradient of the Hessian $D^2 V$.

Finally we write $\nu \ll \mu$ when the measure ν is absolutely continuous with respect to μ and write $\nu \perp \mu$ when they are singular. Throughout the chapter, we denote by $N(m, \Sigma)$ the Gaussian measure on $\mathbf{L}^2(0, 1)$ with mean m and covariance operator Σ . Moreover, the Gaussian measures considered in this chapter will always have the property that, almost

surely, draws from the measure are continuous functions on $[0, 1]$ and thus that point-wise evaluation is well-defined. Given $h \in \mathbf{L}^2(0, 1)$, define the translation map \mathcal{T}_h by setting $\mathcal{T}_h x = x + h$ for any $x \in \mathbf{L}^2(0, 1)$. Denote by $\mathcal{T}_h^* \mu$ the push-forward measure of a measure μ on $\mathbf{L}^2(0, 1)$ under the map \mathcal{T}_h .

5.3 Kullback-Leibler minimisation

5.3.1 Parametrisation of Gaussian Measures

In this subsection, we describe the parametrisation of the Gaussian measures that we use in our Kullback-Leibler minimisation. To motivate our choice of parametrisation we consider the SDE (5.10). This equation has order-one noise, but with a strong gradient-form drift which will, most of the time, constrain the sample path to the neighbourhood of critical points of V . The size of the neighbourhood will be defined by small fluctuations whose size scales with $\varepsilon^{\frac{1}{2}}$. To capture this behaviour we seek an approximation to (5.10) of the form $x = m + z$, where m is a path connecting x_{\pm} in unit time and where z describes the small fluctuations. We aim to find m from an appropriate class of functions, and z as time-inhomogenous Ornstein-Uhlenbeck process

$$\begin{aligned} dz(t) &= -\varepsilon^{-1} \mathbf{A}(t) z(t) dt + \sqrt{2} dW(t), \\ z(0) &= z(1) = 0. \end{aligned} \tag{5.18}$$

The time-dependent functions (m, \mathbf{A}) become our unknowns. For subsequent discussions, we require $m \in \mathbf{H}_{\pm}^1(0, 1)$. For \mathbf{A} we assume that $\mathbf{A} \in \mathbf{H}^1(0, 1)$, i.e. $\mathbf{A} \in H^1(0, 1; \mathbf{R}^{d \times d})$ and $\mathbf{A}(t)$ is symmetric for any $t \in (0, 1)$. The symmetry property will simplify the calculation of the change of measures below, and will also be helpful in estimating the Green's functions used to show the Γ -convergence in Section 5.4.

Let $\bar{\nu}_{\varepsilon}$ be the distribution of the process z defined by (5.18) and let $\bar{\mu}_0$ be the corresponding Brownian bridge (with $\mathbf{A} = 0$). The lemma below shows that $\bar{\nu}_{\varepsilon}$ is a centred Gaussian with the covariance operator given by the inverse Schrödinger operator $\Sigma_{\varepsilon} := 2(-\partial_t^2 + \mathbf{B}_{\varepsilon})^{-1}$ with $\mathbf{B}_{\varepsilon} = \varepsilon^{-2} \mathbf{A}^2 - \varepsilon^{-1} \mathbf{A}'$. Here \mathbf{A}' denotes the time-derivative of the matrix \mathbf{A} and $2(-\partial_t^2 + \mathbf{B}_{\varepsilon})^{-1}$ is the inverse of the Schrödinger operator $\frac{1}{2}(-\partial_t^2 + \mathbf{B}_{\varepsilon})$ with Dirichlet boundary condition. Let $\mathbf{M}_{\varepsilon}(t; s)$ be the fundamental matrix satisfying

$$\frac{d}{dt} \mathbf{M}_{\varepsilon}(t, s) = -\varepsilon^{-1} \mathbf{A}(t) \mathbf{M}_{\varepsilon}(t, s), \quad \mathbf{M}_{\varepsilon}(s, s) = \mathbf{I}_d. \tag{5.19}$$

Lemma 5.3.1. *Let $\mathbf{A} \in \mathbf{H}^1(0, 1)$. Then the Radon-Nikodym density of $\bar{\nu}_{\varepsilon}$ with respect to*

$\bar{\mu}_0$ is given by

$$\frac{d\bar{\nu}_\varepsilon}{d\bar{\mu}_0}(z) = \frac{1}{Z_{\bar{\nu},\varepsilon}} \exp\left(-\frac{1}{4} \int_0^1 z(t)^T \mathbf{B}_\varepsilon(t) z(t) dt\right) \quad (5.20)$$

where $\mathbf{B}_\varepsilon = \varepsilon^{-2} \mathbf{A}^2 - \varepsilon^{-1} \mathbf{A}'$ and the normalisation constant

$$Z_{\bar{\nu},\varepsilon} = \exp\left(-\frac{1}{2\varepsilon} \int_0^1 \text{Tr}(\mathbf{A}(t)) dt\right) \cdot \left(\int_0^1 \bar{\mathbf{M}}_\varepsilon(t) \bar{\mathbf{M}}_\varepsilon^T(t) dt\right)^{-1/2}, \quad (5.21)$$

where $\bar{\mathbf{M}}_\varepsilon(t) = \mathbf{M}_\varepsilon(1, t)$. It follows that $\bar{\nu}_\varepsilon = N(0, 2(-\partial_t^2 + \mathbf{B}_\varepsilon)^{-1})$.

Proof. Let z be the unconditioned Ornstein-Uhlenbeck process that satisfies

$$dz(t) = -\varepsilon^{-1} \mathbf{A}(t) z(t) dt + \sqrt{2} dW(t), \quad z(0) = 0. \quad (5.22)$$

Denote by $\tilde{\nu}_\varepsilon$ the law of $z(t), t \in [0, 1]$ solving (5.22) and by $\tilde{\mu}_0$ the law of the process $\sqrt{2}W(t)$. It follows from Girsanov's theorem that

$$\frac{d\tilde{\nu}_\varepsilon}{d\tilde{\mu}_0}(z) = \exp\left(-\frac{1}{2\varepsilon} \int_0^1 \mathbf{A}(t) z(t) \cdot dz(t) - \frac{1}{4\varepsilon^2} \int_0^1 |\mathbf{A}(t) z(t)|^2 dt\right). \quad (5.23)$$

Simplifying the exponent on the right side of the above by Itô's formula gives

$$\frac{d\tilde{\nu}_\varepsilon}{d\tilde{\mu}_0}(z) = \exp\left(-\frac{1}{4} \int_0^1 z(t)^T \mathbf{B}_\varepsilon(t) z(t) dt + \frac{1}{2\varepsilon} \int_0^1 \text{Tr}(\mathbf{A}(t)) dt - \frac{1}{4\varepsilon} z(1)^T \mathbf{A}(1) z(1)\right). \quad (5.24)$$

After conditioning on $z(1) = 0$ and using [112, Lemma 5.3], (5.20) follows from (5.24). We now calculate the normalisation constant $Z_{\bar{\nu},\varepsilon}$. Let ρ_1 be the density of the distribution of $z(1)$ under the measure $\tilde{\nu}_\varepsilon$. Let $\tilde{\mu}_y$ be law of the conditioned process $(\sqrt{2}W(t) | \sqrt{2}W(1) = y)$. From (5.24), one can see that for any bounded measurable function $f : \mathbf{R}^d \rightarrow \mathbf{R}$,

$$\begin{aligned} \mathbb{E}^{\rho_1}[f(z(1))] &= \mathbb{E}^{\tilde{\nu}_\varepsilon}[f(z(1))] \\ &= \mathbb{E}^{\tilde{\mu}_0} \left[\exp\left(-\frac{1}{4} \int_0^1 z(t)^T \mathbf{B}_\varepsilon(t) z(t) dt\right) \right. \\ &\quad \times \exp\left(\frac{1}{2\varepsilon} \int_0^1 \text{Tr}(\mathbf{A}(t)) dt - \frac{1}{4\varepsilon} z(1)^T \mathbf{A}(1) z(1)\right) f(z(1)) \Big] \\ &= \frac{1}{(4\pi)^{d/2}} \int_{\mathbf{R}^d} \exp\left(\frac{1}{2\varepsilon} \int_0^1 \text{Tr}(\mathbf{A}(t)) dt - \frac{1}{4\varepsilon} y^T \mathbf{A}(1) y - \frac{1}{4} |y|^2\right) f(y) \\ &\quad \times \mathbb{E}^{\tilde{\mu}_y} \left[\exp\left(-\frac{1}{4} \int_0^1 z(t)^T \mathbf{B}_\varepsilon(t) z(t) dt\right) \right] dy, \end{aligned} \quad (5.25)$$

where we have used the fact that $z(1) \sim N(0, 2 \cdot \mathbf{I}_d)$ when z is distributed according to $\tilde{\mu}_0$. Then we can read from (5.25) that

$$\rho_1(0) = \mathbb{E}^{\tilde{\mu}_0} \left[\exp \left(-\frac{1}{4} \int_0^1 z(t)^T \mathbf{B}_\varepsilon(t) z(t) dt \right) \right] \exp \left(\frac{1}{2\varepsilon} \int_0^1 \text{Tr}(\mathbf{A}(t)) dt \right) \frac{1}{(4\pi)^{d/2}}. \quad (5.26)$$

On the other hand, we know from Appendix 5.7.2 that the solution $z(t)$ of (5.22) can be represented as

$$z(t) = \sqrt{2} \int_0^t \mathbf{M}_\varepsilon(t, s) dW(s),$$

where \mathbf{M}_ε is the fundamental matrix (see Definition 5.7.3). In particular, by Itô's isometry the random variable $z(1)$ is a centred Gaussian with covariance

$$\mathbb{E}[z(1)z(1)^T] = 2 \int_0^1 \overline{\mathbf{M}}_\varepsilon(t) \overline{\mathbf{M}}_\varepsilon(t)^T dt,$$

where $\overline{\mathbf{M}}_\varepsilon(t) = \mathbf{M}_\varepsilon(1, t)$. Therefore we obtain an alternative expression for ρ_1 , namely

$$\rho_1(0) = \frac{1}{(4\pi)^{d/2}} \left[\det \left(\int_0^1 \overline{\mathbf{M}}_\varepsilon(t) \overline{\mathbf{M}}_\varepsilon(t)^T dt \right) \right]^{-\frac{1}{2}}. \quad (5.27)$$

Comparing the expressions (5.26) and (5.27) yields (5.21). Finally, by the same arguments used in the proof of [187, Lemma C.1], one can see that $\bar{\nu}_\varepsilon = N(0, 2(-\partial_t^2 + \mathbf{B}_\varepsilon)^{-1})$. \square

We remark that the covariance operator $\Sigma_\varepsilon = 2(-\partial_t^2 + \mathbf{B}_\varepsilon)^{-1}$ is bounded from $\mathbf{L}^2(0, 1)$ to $\mathbf{H}^2(0, 1)$ and is trace-class on $\mathbf{L}^2(0, 1)$; see Lemma 5.7.11 and Remark 5.7.12. The sample paths z are almost surely continuous and the covariances are given by

$$\mathbb{E}^{\bar{\nu}_\varepsilon}[z(t)z(s)^T] = 2\mathbf{G}_\varepsilon(t, s), \quad t, s \in [0, 1]. \quad (5.28)$$

Here $\mathbf{G}_\varepsilon(t, s)$ is the Green's tensor (fundamental matrix) of the elliptic operator $(-\partial_t^2 + \mathbf{B}_\varepsilon)$ under Dirichlet boundary conditions, i.e. for any $s \in (0, 1)$,

$$\begin{aligned} (-\partial_t^2 + \varepsilon^{-2} \mathbf{A}^2(\cdot) - \varepsilon^{-1} \mathbf{A}'(\cdot)) \mathbf{G}_\varepsilon(\cdot, s) &= \delta(\cdot - s) \cdot \mathbf{I}_d, \\ \mathbf{G}_\varepsilon(0, s) &= \mathbf{G}_\varepsilon(1, s) = 0. \end{aligned} \quad (5.29)$$

With a description of the centred fluctuation process z in hand we now move on to discuss the non-centred process $x = m + z$, whose law is denoted by ν_ε . It is clear that $\nu_\varepsilon = N(m, \Sigma_\varepsilon)$. Because of (5.18), ν_ε can also be viewed as the law of the following

conditioned Ornstein-Uhlenbeck process

$$\begin{aligned} dx(t) &= (m'(t) - \varepsilon^{-1} \mathbf{A}(t)(x(t) - m(t))) dt + \sqrt{2} dW(t), \\ x(0) &= x_-, \quad x(1) = x_+. \end{aligned} \quad (5.30)$$

Hence the Gaussian measure ν_ε is parametrised by the pair of functions (m, \mathbf{A}) . To conclude, recalling the space $\mathcal{H}_a = \mathbf{H}_\pm^1(0, 1) \times \mathbf{H}_a^1(0, 1)$, we define the family of Gaussian measures as

$$\mathcal{A} = \left\{ N(m, 2(-\partial_t^2 + \mathbf{B}_\varepsilon)^{-1}) : (m, \mathbf{A}) \in \mathcal{H} \right\} \quad (5.31)$$

where $\mathbf{B}_\varepsilon = \varepsilon^{-2} \mathbf{A}^2 - \varepsilon^{-1} \mathbf{A}'$. For $a > 0$, we denote by \mathcal{A}_a the set of Gaussian measures defined in the same way as (5.31) but with \mathcal{H} replaced by \mathcal{H}_a .

5.3.2 Calculations of Kullback-Leibler Divergence

To quantify the closeness of probability measures, we use the Kullback-Leibler divergence, or relative entropy. Given two probability measures ν and μ , with ν absolutely continuous with respect to μ , the Kullback-Leibler divergence of ν and μ is

$$D_{\text{KL}}(\nu || \mu) = \mathbb{E}^\nu \log \left(\frac{d\nu}{d\mu} \right)$$

where \mathbb{E}^ν denotes the expectation taken with respect to the measure ν ; if ν is not absolutely continuous with respect to μ , then the Kullback-Leibler divergence is defined as $+\infty$. Sometimes it is convenient to evaluate the Kullback-Leibler divergence through a reference measure μ_0 . If the measures μ, ν and μ_0 are mutually equivalent, then the Kullback-Leibler divergence can be expressed as

$$D_{\text{KL}}(\nu || \mu) = \mathbb{E}^\nu \log \left(\frac{d\nu}{d\mu_0} \right) - \mathbb{E}^\nu \log \left(\frac{d\mu}{d\mu_0} \right). \quad (5.32)$$

In this section, we calculate the Kullback-Leibler divergence between the non-Gaussian measure μ_ε (defined by (5.17)) and the parametrised Gaussian measure $\nu_\varepsilon = N(m, \Sigma_\varepsilon)$. Recall that $\bar{\nu}_\varepsilon$ is the law of the time-inhomogeneous Ornstein-Uhlenbeck process (5.18). Recall also that μ_0 is the law of the Brownian bridge process corresponding to vanishing drift in the SDE (5.10). It is clear that $\mu_0 = N(m_0, 2(-\partial_t^2)^{-1})$ with $m_0(t) = x_-(1-t) + x_+t$. In order to evaluate the above Kullback-Leibler divergence by using (5.32), we need to calculate the Radon-Nikodym derivative $d\nu_\varepsilon/d\mu_0$.

Lemma 5.3.2. *Let $m \in \mathbf{H}_\pm^1(0, 1)$ and $\mathbf{A} \in \mathbf{H}^1(0, 1)$. Then the Radon-Nikodym density of*

ν_ε with respect to μ_0 is given by

$$\frac{d\nu_\varepsilon}{d\mu_0}(x) = \frac{1}{Z_{\nu,\varepsilon}} \exp(-\Phi_{\nu,\varepsilon}(x)) \quad (5.33)$$

where

$$\begin{aligned} \Phi_{\nu,\varepsilon}(x) &= \frac{1}{4} \int_0^1 (x(t) - m(t))^T \mathbf{B}_\varepsilon(t) (x(t) - m(t)) dt \\ &\quad - \frac{1}{2} \int_0^1 m'(t) \cdot dx(t) + \frac{1}{4} \int_0^1 |m'(t)|^2 dt. \end{aligned} \quad (5.34)$$

and the normalisation constant

$$Z_{\nu,\varepsilon} = \exp\left(\frac{|x_1 - x_0|^2}{4}\right) \cdot \exp\left(-\frac{1}{2\varepsilon} \int_0^1 \text{Tr}(\mathbf{A}(t)) dt\right) \cdot \left(\int_0^1 \overline{\mathbf{M}}_\varepsilon(t) \overline{\mathbf{M}}_\varepsilon^T(t) dt\right)^{-1/2}, \quad (5.35)$$

where $\overline{\mathbf{M}}_\varepsilon(t) = \mathbf{M}_\varepsilon(1, t)$.

Proof. First by definitions of $\bar{\nu}_\varepsilon$ and $\bar{\mu}_0$, we know that $\nu_\varepsilon = \mathcal{T}_m^* \bar{\nu}_\varepsilon$ and $\mu_0 = \mathcal{T}_{m_0}^* \bar{\mu}_0$. Then we have

$$\frac{d\nu_\varepsilon}{d\mu_0}(x) = \frac{d\mathcal{T}_m^* \bar{\nu}_\varepsilon}{d\mathcal{T}_{m_0}^* \bar{\mu}_0}(x) = \frac{d\mathcal{T}_m^* \bar{\nu}_\varepsilon}{d\mathcal{T}_m^* \bar{\mu}_0}(x) \cdot \frac{d\mathcal{T}_m^* \bar{\mu}_0}{d\mathcal{T}_{m_0}^* \bar{\mu}_0}(x). \quad (5.36)$$

Observe that for any Borel set $A \subset \mathbf{L}^2(0, 1)$,

$$\mathcal{T}_m^* \bar{\nu}_\varepsilon(A) = \bar{\nu}_\varepsilon(A - m) = \mathbb{E}^{\bar{\mu}_0} \left[\frac{d\bar{\nu}_\varepsilon}{d\bar{\mu}_0}(x) \mathbf{1}_{A-m}(x) \right] = \mathbb{E}^{\mathcal{T}_m^\# \bar{\mu}_0} \left[\frac{d\bar{\nu}_\varepsilon}{d\bar{\mu}_0}(x - m) \mathbf{1}_A(x) \right].$$

This together with Lemma 5.3.1 implies that

$$\begin{aligned} \frac{d\mathcal{T}_m^* \bar{\nu}_\varepsilon}{d\mathcal{T}_{m_0}^* \bar{\mu}_0}(x) &= \frac{d\bar{\nu}_\varepsilon}{d\bar{\mu}_0}(x - m). \\ &= \frac{1}{Z_{\bar{\nu},\varepsilon}} \exp\left(-\frac{1}{4} \int_0^1 (x(t) - m(t))^T \mathbf{B}_\varepsilon(t) (x(t) - m(t)) dt\right). \end{aligned} \quad (5.37)$$

Since $m \in \mathbf{H}_\pm^1(0, 1)$, $m - m_0 \in \mathbf{H}_0^1(0, 1)$ and hence $\mathcal{T}_m^* \bar{\mu}_0 \ll \mathcal{T}_{m_0}^* \bar{\mu}_0$. Furthermore, by the Cameron-Martin formula [21] we have

$$\begin{aligned} \frac{d\mathcal{T}_m^* \bar{\mu}_0}{d\mathcal{T}_{m_0}^* \bar{\mu}_0}(x) &= \exp\left(\frac{1}{2} \int_0^1 (m'(t) - m_0'(t)) \cdot d(x(t) - m(t))\right. \\ &\quad \left. - \frac{1}{4} \int_0^1 |m'(t) - m_0'(t)|^2 dt\right). \end{aligned} \quad (5.38)$$

Recall that $m_0(t) = x_-(1-t) + x_+t$. Using the fact that $x(0) = x_-$, $x(1) = x_+$ when x is distributed according to $\mathcal{T}_m^* \bar{\mu}_0$ (or $\mathcal{T}_{m_0}^* \bar{\mu}_0$), we can simplify the exponent of above as follows:

$$\begin{aligned}
& \frac{1}{2} \int_0^1 (m'(t) - m'_0(t)) \cdot d(x(t) - m_0(t)) - \frac{1}{4} \int_0^1 |m'(t) - m'_0(t)|^2 dt \\
&= \frac{1}{2} \int_0^1 m'(t) \cdot dx(t) - \frac{1}{4} \int_0^1 |m'(t)|^2 dt - \frac{1}{2} \int_0^1 m'_0(t) \cdot d(x(t) - m_0(t)) \\
&\quad - \frac{1}{4} \int_0^1 |m'_0(t)|^2 dt \\
&= \frac{1}{2} \int_0^1 m'(t) \cdot dx(t) - \frac{1}{4} \int_0^1 |m'(t)|^2 dt - \frac{|x_+ - x_-|^2}{4}.
\end{aligned} \tag{5.39}$$

Hence one can obtain (5.33) from (5.36)-(5.39) where the normalisation constant

$$Z_{\nu, \varepsilon} = Z_{\bar{\nu}, \varepsilon} \cdot \exp\left(\frac{|x_+ - x_-|^2}{4}\right).$$

This together with (5.21) implies (5.35). \square

According to the definition of μ_ε (given by (5.17)), Lemma 5.3.2 and the expression (5.32) for the Kullback-Leibler divergence we obtain that

$$D_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon) = \tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon) - \frac{|x_1 - x_0|^2}{4} + \log(Z_{\mu, \varepsilon}), \tag{5.40}$$

where

$$\begin{aligned}
\tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon) &= \frac{1}{2\varepsilon^2} \mathbb{E}^{\bar{\nu}_\varepsilon} \int_0^1 \Psi_\varepsilon(z(t) + m(t)) dt + \frac{1}{4} \int_0^1 |m'(t)|^2 dt \\
&\quad - \frac{1}{4} \mathbb{E}^{\bar{\nu}_\varepsilon} \left[\int_0^1 z(t)^T \mathbf{B}_\varepsilon(t) z(t) dt \right] + \frac{1}{2\varepsilon} \int_0^1 \text{Tr}(\mathbf{A}(t)) dt \\
&\quad + \frac{1}{2} \log \left(\det \left(\int_0^1 \bar{\mathbf{M}}_\varepsilon(t) \bar{\mathbf{M}}_\varepsilon(t)^T dt \right) \right).
\end{aligned} \tag{5.41}$$

Here $\bar{\nu}_\varepsilon = N(0, 2(-\partial_t^2 + \mathbf{B}_\varepsilon)^{-1})$ and $\bar{\mathbf{M}}_\varepsilon(t) = \mathbf{M}_\varepsilon(1, t)$ with \mathbf{M}_ε defined by (5.19). The form of $\tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$ is interesting: the first two terms comprise a “fattened” version of the Onsager-Machlup functions (5.9), where the fattening is characterised by the entropic fluctuations of the process z . The remaining terms penalise those entropic contributions. This characterisation will be particularly clear in the small noise limit – see the discussion in Section 5.5.

5.3.3 Variational Problem

Recall the set of Gaussian measures

$$\mathcal{A} = \left\{ N(m, 2(-\partial_t^2 + \mathbf{B}_\varepsilon)^{-1}) : (m, \mathbf{A}) \in \mathcal{H} \right\}$$

where $\mathbf{B}_\varepsilon = \varepsilon^{-2}\mathbf{A}^2 - \varepsilon^{-1}\mathbf{A}'$ and that the set \mathcal{A}_a is defined in the same way with \mathcal{H} replaced by \mathcal{H}_a for some $a > 0$. Given the measure μ_ε defined by (5.17), i.e. the law of transition paths, we aim to find optimal Gaussian measures ν_ε from \mathcal{A} or \mathcal{A}_a minimising the Kullback-Leibler divergence $D_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$. To that end, first in view of (5.40), the constants $\frac{|x_1 - x_0|^2}{4}$ and $\log(Z_{\mu, \varepsilon})$ can be neglected in the minimisation process since they do not depend on the choice of ν_ε . Hence we are only concerned with minimising the modified Kullback-Leibler divergence $\tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$. Furthermore, instead of minimising $\tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$, we consider the variational problem

$$\inf_{\nu \in \mathcal{A}} \left(\varepsilon \tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon) + \varepsilon^\gamma \|\mathbf{A}\|_{\mathbf{H}^1(0,1)}^2 \right), \quad (5.42)$$

where $\gamma > 0$ and \mathcal{A} is given by (5.31). We will also study the minimisation problem over the set \mathcal{A}_a . The reasons why the problem (5.42) is of interest to us are the following. First, multiplying $\tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$ by ε does not change the minimisers. Yet after this scaling the m -dependent terms of $\tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$ (the first two terms on the right hand side of (5.41)) and the \mathbf{A} -dependent terms (middle line of (5.41)) are well-balanced since they are all order one quantities with respect to ε . Moreover, the regularisation term $\varepsilon^\gamma \|\mathbf{A}\|_{\mathbf{H}^1(0,1)}^2$ is necessary because the matrix \mathbf{B}_ε , along any infimising sequence for $\varepsilon \tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$, will only converge weakly and the minimiser may not be attained in \mathcal{A} . This issue is illustrated in [187, Example 3.8 and Example 3.9] and a similar regularisation is used there.

Remark 5.3.3. *The normalisation constant $Z_{\mu, \varepsilon}$ in (5.40) is dropped in our minimisation problem. This is one of the advantages of quantifying measure approximations by means of the Kullback-Leibler divergence. However, understanding the asymptotic behaviour of $Z_{\mu, \varepsilon}$ in the limit $\varepsilon \rightarrow 0$ is quite important, even though this is difficult. In particular, it allows us to study the asymptotic behaviour of the scaled Kullback-Leibler divergence $\varepsilon D_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$, whereby quantitative information on the quality of the Gaussian approximation in the small temperature limit can be extracted. In the next section we study behaviour of the minimisers of the functional defined in (5.42) in the limit $\varepsilon \rightarrow 0$; we postpone study of $\varepsilon D_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$, which requires analysis of $Z_{\mu, \varepsilon}$ in the limit $\varepsilon \rightarrow 0$, to future work. \square*

Remark 5.3.4. *We choose the small weight ε^γ with some $\gamma > 0$ in front of the regularisation term with the aim of weakening the contribution from the regularisation so that it disappears in the limit $\varepsilon \rightarrow 0$. For the study of the Γ -limit of F_ε , we will consider $\gamma \in (0, \frac{1}{2})$; see*

Theorem 5.4.5 in the next section. \square

Remark 5.3.5. The Kullback-Leibler divergence is not symmetric in its arguments. We do not study $\tilde{D}_{KL}(\mu_\varepsilon || \nu_\varepsilon)$ because minimisation of this functional over the class of Gaussian measures leads simply to moment matching and this is not appropriate for problems with multiple minimisers, see [19, Section 10.7]. \square

The following theorem establishes the existence of minimisers for the problem (5.42).

Theorem 5.3.6. Given the measure μ_ε defined by (5.17) with fixed $\varepsilon > 0$. There exists at least one measure $\nu \in \mathcal{A}$ (or \mathcal{A}_a) minimising the functional

$$\nu \mapsto \varepsilon \tilde{D}_{KL}(\nu || \mu_\varepsilon) + \varepsilon^\gamma \|\mathbf{A}\|_{\mathbf{H}^1(0,1)}^2 \quad (5.43)$$

over \mathcal{A} (or \mathcal{A}_a).

Proof. We only prove the theorem for the case where the minimising problem is defined over \mathcal{A}_a since the other case can be treated in the same manner. First we show that the infimum of (5.43) over \mathcal{A}_a is finite for any fixed $\varepsilon > 0$. In fact, consider $\mathbf{A}^* = a \cdot \mathbf{I}_d$ with $a > 0$ and m^* being any fixed function in $\mathbf{H}_\pm^1(0,1)$. Then we show that $F(m^*, \mathbf{A}^*)$ is finite. For this, by the formula (5.41), we only need to show that

$$\mathbb{E}^{\bar{\nu}_\varepsilon} \int_0^1 \Psi_\varepsilon(z(t) + m^*(t)) dt < \infty.$$

Since $\mathbf{A}^* = a \cdot \mathbf{I}_d$, from (5.28) one can see that $z(t) \sim N(0, 2\mathbf{G}_\varepsilon(t, t))$ under the measure $\bar{\nu}_\varepsilon$. In addition, it follows from (5.71) that $|\mathbf{G}_\varepsilon(t, t)|_F \leq C\varepsilon$ a.e. on $(0, 1)$ for some $C > 0$. Then from the growth condition (A-4) on Ψ_ε and the fact that $m^* \in \mathbf{L}^\infty(0, 1)$,

$$\begin{aligned} & \mathbb{E}^{\bar{\nu}_\varepsilon} \int_0^1 \Psi_\varepsilon(z(t) + m^*(t)) dt \\ &= \int_0^1 \int_{\mathbf{R}^d} \frac{1}{\sqrt{(4\pi)^d \det(\mathbf{G}_\varepsilon(t, t))}} e^{-\frac{1}{4}x^T \mathbf{G}_\varepsilon(t, t)^{-1}x} \Psi_\varepsilon(x + m^*(t)) dx dt \\ &= \int_0^1 \int_{\mathbf{R}^d} \frac{1}{(4\pi)^{d/2}} e^{-\frac{1}{4}|x|^2} \Psi_\varepsilon\left((\mathbf{G}_\varepsilon(t, t)^{1/2})x + m^*(t)\right) dx dt \\ &\leq C_1 \exp\left(\|m^*\|_{\mathbf{L}^\infty(0,1)}^\alpha\right) \int_{\mathbf{R}^d} e^{-\frac{1}{2}|x|^2 + C_2\varepsilon^\alpha|x|^\alpha} dx < \infty \end{aligned}$$

since $\alpha \in [0, 2)$.

Next, we prove that the minimiser exists. By examining the proof of [187, Theorem 3.10], one can see that the theorem is proved if the following statement is valid: if

a sequence $\{\mathbf{A}_n\} \subset \mathbf{H}_a^1(0, 1)$ satisfies $\sup_n \|\mathbf{A}_n\|_{\mathbf{H}^1(0,1)} < \infty$, then the sequence $\{\mathbf{B}_n\}$ with $B_n = \varepsilon^{-2}\mathbf{A}_n^2 - \varepsilon^{-1}\mathbf{A}'_n$, viewed as multiplication operators, contains a subsequence that converges to $\mathbf{B} = \varepsilon^{-2}\mathbf{A}^2 - \varepsilon^{-1}\mathbf{A}'$ in $\mathcal{L}(\mathbf{H}^\beta, \mathbf{H}^{-\beta})$ for some $\mathbf{A} \in \mathbf{H}_a^1(0, 1)$ and some $\beta \in (0, 1)$. Hence we only need to show that the latter statement is true. In fact, if $\sup_n \|\mathbf{A}_n\|_{\mathbf{H}^1(0,1)} < \infty$, then there exists a subsequence $\{\mathbf{A}_{n_k}\}$ and some $\mathbf{A} \in \mathbf{H}^1(0, 1)$ such that $\mathbf{A}_{n_k} \rightharpoonup \mathbf{A}$ in $\mathbf{H}^1(0, 1)$. By Rellich's compact embedding theorem, $\mathbf{A}_{n_k} \rightarrow \mathbf{A}$ in $\mathbf{L}^2(0, 1)$ and passing to a further subsequence we may assume that $\mathbf{A}_{n_k} \rightarrow \mathbf{A}$ a.e. on $[0, 1]$. This implies that \mathbf{A} is symmetric and $\mathbf{A} \geq a \cdot \mathbf{I}_d$ a.e. and hence $\mathbf{A} \in \mathbf{H}_a^1(0, 1)$. In addition, it is clear that $\mathbf{B}_{n_k} \rightharpoonup \mathbf{B}$ in $\mathbf{L}^2(0, 1)$. According to Lemma 5.7.9, for any $\alpha, \beta > 0$ such that $\beta > \max(\alpha, \alpha/2 + 1/4)$, a matrix-valued function in $\mathbf{H}^{-\alpha}(0, 1)$ can be viewed as a multiplication operator in $\mathcal{L}(\mathbf{H}^\beta, \mathbf{H}^{-\beta})$. Thanks to the compact embedding from $\mathbf{L}^2(0, 1)$ to $\mathbf{H}^{-\alpha}(0, 1)$, we obtain $\mathbf{B}_{n_k} \rightarrow \mathbf{B}$ in $\mathcal{L}(\mathbf{H}^\beta, \mathbf{H}^{-\beta})$. The proof is complete. \square

Remark 5.3.7. *minimisers of (5.43) are not unique in general. The uniqueness issue is outside the scope of this chapter; see more discussions about uniqueness of minimising the Kullback-Leibler divergence in [187, Section 3.4].* \square

5.4 Low Temperature Limit

In this section, we aim to understand the low temperature limit of the best Gaussian approximations discussed in the previous section. This will be done by investigating the Γ -convergence (see Definition 2.4.1) of some energy functional. In fact, consider the following family of functionals:

$$F_\varepsilon(m, \mathbf{A}) := \begin{cases} \varepsilon \tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon) + \varepsilon^\gamma \|\mathbf{A}\|_{\mathbf{H}^1(0,1)}^2, & \text{if } (m, \mathbf{A}) \in \mathcal{H}, \\ \infty, & \text{otherwise in } \mathcal{X} \end{cases} \quad (5.44)$$

on the space $\mathcal{X} = \mathbf{L}^1(0, 1) \times \mathbf{L}^1(0, 1)$. Then minimising (5.43) over \mathcal{A} is equivalent to the following problem

$$\inf_{(m, \mathbf{A}) \in \mathcal{X}} F_\varepsilon(m, \mathbf{A}). \quad (5.45)$$

In order to study the Γ -limit of F_ε , we equip the space \mathcal{X} with a product topology such that the convergence $(m_\varepsilon, \mathbf{A}_\varepsilon) \rightarrow (m, \mathbf{A})$ in \mathcal{X} means that $m_\varepsilon \rightarrow m$ in $\mathbf{L}^1(0, 1)$ and that $\mathbf{A}_\varepsilon \rightharpoonup \mathbf{A}$ in $\mathbf{L}^1(0, 1)$. The reason for choosing the weak topology for \mathbf{A} is that the functional F_ε is coercive under such topology only, see Proposition 5.4.4. Now before we proceed to discussing the Γ -convergence of F_ε , we first state a useful Γ -convergence result

for the classical Ginzburg-Landau functional

$$E_\varepsilon(m) := \begin{cases} \frac{\varepsilon}{4} \int_0^1 |m'(t)|^2 dt + \frac{1}{4\varepsilon} \int_0^1 |\nabla V(m(t))|^2 dt & \text{if } m \in \mathbf{H}_\pm^1(0, 1), \\ \infty, & \text{otherwise in } \mathbf{L}^1(0, 1). \end{cases} \quad (5.46)$$

Notice that in the above definition, any m such that $E_\varepsilon(m)$ is finite should satisfy the Dirichlet boundary conditions $m(0) = x_-$ and $m(1) = x_+$. We also remark that after performing the scaling transformation $t \mapsto \varepsilon^{-1}t$, the functional E_ε coincides with the Freidlin-Wentzell functional S_T (defined in (5.6)) with $T = \varepsilon^{-1}$. Indeed, by rewriting $\tilde{m}(\cdot) = m(\varepsilon^{-1}\cdot)$, one sees that $E_\varepsilon(m) = S_T(\tilde{m})$.

To define the Γ -limit of E_ε , we now introduce some additional notations. Recall that \mathcal{E} defined in (5.11) is the set of critical points of V . For each pair $x_-, x_+ \in \mathcal{E}$, we define the set of transition paths

$$\mathbf{X}(x_-, x_+) := \{m \in \mathbf{BV}(\mathbf{R}) \mid \lim_{t \rightarrow \pm\infty} m(t) = x_\pm \text{ and } m' \in \mathbf{L}^2(\mathbf{R})\},$$

the cost functional

$$\mathcal{J}_T(m) = \frac{1}{4} \int_{-T}^T \left(|m'(t)|^2 + |\nabla V(m(t))|^2 \right) dt, \quad (5.47)$$

and set $\mathcal{J}(m) := \mathcal{J}_\infty(m)$. The minimal transition cost from x_- to x_+ is then defined as

$$\Phi(x_-, x_+) := \inf \{ \mathcal{J}(m) \mid m \in \mathbf{X}(x_-, x_+) \}.$$

It is worth noting that the function $\Phi(x_-, x_+)$ is closely related to the so-called quasi-potential, which plays an important role in large deviation theory. In fact, suppose that $x_-, x_+ \in \mathcal{E}$ and that V satisfies Assumption (5.2.1). Then according to [96, Lemma 3.2], the function $\Phi(x_-, x_+)$ has the following equivalent form:

$$\begin{aligned} & \Phi(x_-, x_+) \\ &= \inf_{T, m} \left\{ \mathcal{J}_T(m) : T > 0, m \in \mathbf{H}^1(-T, T) \text{ and } m(-T) = x_-, m(T) = x_+ \right\}. \end{aligned} \quad (5.48)$$

This definition shows that $\Phi(x_-, x_+)$ coincides with the quasi-potential between x_- and x_+ (as defined in [98, Chapter 4]) up to the additive constant $-\frac{1}{2}(V(x_+) - V(x_-))$.

We also remark that the equivalent formulation (5.48) provides an important ingredient for proving the Γ -convergence of E_ε ; see e.g. [25, 96]. Given $x_\pm \in \mathcal{E}$, if either x_- or x_+ is a local minimum or maximum of potential V and if V satisfies (A-1)-(A-3) of Assumption 5.2.1, it was shown in [189, Lemma 2.1] that the infimum $\Phi(x_-, x_+)$ is attained

by the heteroclinic orbits m_* of the Hamiltonian system

$$m_*''(t) - D^2V(m_*)\nabla V(m_*) = 0, \quad \lim_{t \rightarrow \pm\infty} m(t) = x_{\pm}.$$

In this case,

$$\Phi(x_-, x_+) = \frac{1}{2}|V(x_+) - V(x_-)|. \quad (5.49)$$

Denote by $\mathbf{BV}(0, 1; \mathcal{E})$ the set of functions in $\mathbf{BV}(0, 1)$ taking values in \mathcal{E} a.e. on $[0, 1]$. For any $u \in \mathbf{BV}(0, 1; \mathcal{E})$, let $J(u)$ be the set of jump points of u on $(0, 1)$, and let $u(t^{\pm})$ the left and right sided limits of u at time $t \in [0, 1]$. The following lemma, concerning the compactness of E_{ε} , will be very useful in identifying its Γ -limit. Its proof can be found in [149, Theorem 1.2].

Lemma 5.4.1. *Assume that the potential V satisfies (A-1)-(A-3). Let $\varepsilon_n \rightarrow 0$ and let $\{m_n\} \subset \mathbf{H}_{\pm}^1(0, 1)$ be such that*

$$\limsup_{n \rightarrow \infty} E_{\varepsilon_n}(m_n) < \infty.$$

Then there exists a subsequence $\{m_{n_k}\}$ of $\{m_n\}$ and an $m \in \mathbf{BV}(0, 1; \mathcal{E})$ such that $m_{n_k} \rightarrow m$ in $\mathbf{L}^1(0, 1)$ as $k \rightarrow \infty$.

We remark that we incorporate the boundary conditions $m_n(0) = x_-$, $m_n(1) = x_+$ in the statement of the lemma since $m_n \in \mathbf{H}_{\pm}^1(0, 1)$. The following Proposition identifies the Γ -limit of E_{ε} with respect to \mathbf{L}^1 -topology; this is based upon Lemma 5.4.1 and the standard Modica-Mortola type arguments (see [12, 171, 189]). The proof is given in Appendix 5.7.4. The same Γ -convergence result was claimed in [189], but the proof there was actually carried out with respect to the topology in the space of functions of bounded variations.

Proposition 5.4.2. *Assume that V satisfies the conditions (A-1)-(A-3), the Γ -limit of E_{ε} is*

$$E(m) := \begin{cases} \Phi(x_-, m(0^+)) + \sum_{\tau \in J(m)} \Phi(m(\tau^-), m(\tau^+)) \\ \quad + \Phi(m(1^-), x_+) & \text{if } m \in \mathbf{BV}(0, 1; \mathcal{E}), \\ +\infty & \text{otherwise in } \mathbf{L}^1(0, 1). \end{cases} \quad (5.50)$$

5.4.1 Main Results

This subsection presents the main results about the Γ -convergence of the functional F_{ε} ; the proofs will be presented in the next section. Roughly speaking, our arguments indicate that

the Γ -limit of F_ε on \mathcal{X} should be

$$F(m, \mathbf{A}) := E(m) + \frac{1}{4} \int_0^1 (D^2 V(m(t)) - |\mathbf{A}(t)|)^2 : |\mathbf{A}^{-1}(t)| dt \quad (5.51)$$

where $E(m)$ is defined by (5.50). Recall that $\mathbf{A} : \mathbf{B} = \text{Tr}(\mathbf{A}\mathbf{B}^T)$ and that $|\mathbf{A}| = \mathbf{P}^T |\mathbf{\Lambda}| \mathbf{P}$ with $\mathbf{A} = \mathbf{P}^T \mathbf{\Lambda} \mathbf{P}$. However, for technical reasons, we are only able to prove the claim under the condition that the matrix \mathbf{A} is positive definite; see Remark 5.4.8. To make this clear, let us first redefine F_ε to be

$$F_\varepsilon(m, \mathbf{A}) := \begin{cases} \varepsilon \tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon) + \varepsilon^\gamma \|\mathbf{A}\|_{\mathbf{H}^1(0,1)}^2, & \text{if } (m, \mathbf{A}) \in \mathcal{H}_a, \\ \infty, & \text{otherwise in } \mathcal{X}_a \end{cases} \quad (5.52)$$

with some $a > 0$. Then we can show that F_ε as defined in (5.52) Γ -converges to F defined by (5.51) on the space \mathcal{X}_a for any $a > 0$; see Theorem 5.4.5. Recall that $\mathcal{X}_a = \mathbf{L}^1(0, 1) \times \mathbf{L}_a^1(0, 1)$ and that convergence of (m_n, \mathbf{A}_n) in \mathcal{X}_a means that the m_n converge strongly in $\mathbf{L}^1(0, 1)$ and the \mathbf{A}_n converge weakly in $\mathbf{L}_a^1(0, 1)$.

By the definition of F_ε (by (5.52)) and the expression (5.40) for $\tilde{D}_{\text{KL}}(\nu_\varepsilon || \mu_\varepsilon)$, we can write

$$F_\varepsilon(m, \mathbf{A}) = F_\varepsilon^{(1)}(m, \mathbf{A}) + F_\varepsilon^{(2)}(\mathbf{A}) + \varepsilon^\gamma \|\mathbf{A}\|_{\mathbf{H}^1(0,1)}^2 \quad (5.53)$$

for $(m, \mathbf{A}) \in \mathcal{H}_a$ where

$$\begin{aligned} F_\varepsilon^{(1)}(m, \mathbf{A}) &:= \frac{\varepsilon}{4} \int_0^1 |m'(t)|^2 dt + \frac{1}{2\varepsilon} \mathbb{E}^{\bar{\nu}_\varepsilon} \left[\int_0^1 \Psi_\varepsilon(z(t) + m(t)) dt \right], \\ F_\varepsilon^{(2)}(\mathbf{A}) &:= -\frac{\varepsilon}{4} \mathbb{E}^{\bar{\nu}_\varepsilon} \left[\int_0^1 z(t)^T \mathbf{B}_\varepsilon(t) z(t) dt \right] + \frac{1}{2} \int_0^1 \text{Tr}(\mathbf{A}(t)) dt \\ &\quad + \frac{\varepsilon}{2} \log \left(\det \left(\int_0^1 \overline{\mathbf{M}}_\varepsilon(t) \overline{\mathbf{M}}_\varepsilon(t)^T dt \right) \right), \end{aligned} \quad (5.54)$$

where Ψ_ε is given by (5.8) and $\overline{\mathbf{M}}_\varepsilon$ is defined by (5.19). To identify the Γ -limit of F_ε , we need to study the liminf or limsup of the sequence $\{F_\varepsilon(m_\varepsilon, \mathbf{A}_\varepsilon)\}$ with $m_\varepsilon \in \mathbf{H}_\pm^1(0, 1)$ and $\mathbf{A}_\varepsilon \in \mathbf{H}_a^1(0, 1)$. This is non-trivial in our case, mainly because the functional F_ε depends on m and \mathbf{A} in an implicit manner through the two expectation terms. Therefore in the first step we shall simplify F_ε . The following proposition examines the limiting behaviour of the functional F_ε from which a simplified and more explicit expression is obtained.

Proposition 5.4.3. *Let $(m_\varepsilon, \mathbf{A}_\varepsilon) \in \mathcal{H}_a$. Assume that for some $\gamma \in (0, \frac{1}{2})$,*

$$\limsup_{\varepsilon \rightarrow 0} \varepsilon^\gamma \|\mathbf{A}_\varepsilon\|_{\mathbf{H}^1(0,1)}^2 < \infty \quad \text{and} \quad \limsup_{\varepsilon \rightarrow 0} \|m_\varepsilon\|_{\mathbf{L}^\infty(0,1)} < \infty.$$

Then for $\varepsilon > 0$ small enough we have

$$\begin{aligned} F_\varepsilon(m_\varepsilon, \mathbf{A}_\varepsilon) &= E_\varepsilon(m_\varepsilon) + \frac{1}{4} \int_0^1 (D^2 V(m_\varepsilon(t)) - \mathbf{A}_\varepsilon(t))^2 : \mathbf{A}_\varepsilon^{-1}(t) dt \\ &\quad + \int_0^1 (D^3 V(m_\varepsilon(t)) \cdot \nabla V(m_\varepsilon(t))) : \mathbf{A}_\varepsilon^{-1}(t) dt + \varepsilon^\gamma \|\mathbf{A}_\varepsilon\|_{\mathbf{H}^1(0,1)}^2 + \mathcal{O}(\varepsilon^{\frac{1}{2}}). \end{aligned} \quad (5.55)$$

The proof of Proposition 5.4.3 requires several technical lemmas and is referred to Section 5.6.3. The basic idea for proving Proposition 5.4.3 is as follows. First one can express the expectation term in $F_\varepsilon^{(2)}(\mathbf{A}_\varepsilon)$ in terms of the Dirichlet Green's tensor of some Schrödinger operator (see (5.59)). A careful asymptotic analysis of this Green's tensor implies that

$$F_\varepsilon^{(2)}(\mathbf{A}_\varepsilon) \approx \frac{1}{4} \int_0^1 \text{Tr}(\mathbf{A}_\varepsilon(t)) dt, \quad (5.56)$$

see Corollary 5.6.2 for the precise statement. For the expectation term in $F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon)$, we approximate $\Psi_\varepsilon(X)$ by its second order Taylor expansion around the mean m_ε . The zero order term of the expansion is $\Psi_\varepsilon(m_\varepsilon) = \frac{1}{2} |\nabla V(m_\varepsilon)|^2 - \varepsilon \Delta V(m_\varepsilon)$. Then $E_\varepsilon(m_\varepsilon)$ is obtained by combining the term $\frac{\varepsilon}{4} \int_0^1 |m'(t)|^2 dt$ in $F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon)$ with the integral over $\frac{1}{4\varepsilon} |\nabla V(m_\varepsilon)|^2$. Additionally, the Itô correction term $-\varepsilon \Delta V(m_\varepsilon)$, which is the other zero order term of the Taylor expansion, can be combined with one of the second order terms of the expansion and (5.56) to complete the full quadratic term in (5.55).

As a consequence of Proposition 5.4.3, we get the following compactness result for the functional F_ε .

Proposition 5.4.4. *Let $\varepsilon_n \rightarrow 0$ and let $\{(m_n, \mathbf{A}_n)\}$ be a sequence in \mathcal{H}_a such that*

$$\limsup_n F_{\varepsilon_n}(m_n, \mathbf{A}_n) < \infty.$$

Then there exists a subsequence $\{(m_{n_k}, \mathbf{A}_{n_k})\}$ of $\{(m_n, \mathbf{A}_n)\}$ such that $m_{n_k} \rightarrow m$ in $\mathbf{L}^1(0, 1)$ and $\mathbf{A}_{n_k} \rightharpoonup \mathbf{A}$ in $\mathbf{L}^1(0, 1)$ with $m \in \mathbf{BV}(0, 1; \mathcal{E})$ and $\mathbf{A} \in \mathbf{L}_a^1(0, 1)$.

This compactness result is slightly weaker than the usual compactness property relevant to Γ -convergence (see e.g. the conclusion in Lemma 5.4.1), because only weak convergence is obtained for the variable \mathbf{A} . Building upon the Γ -convergence result of

E_ε , Proposition 5.4.3 and Proposition 5.4.4, the following main theorem establishes the Γ -convergence of F_ε .

Theorem 5.4.5. *Suppose that V satisfies the assumptions (A-1)-(A-6). Let $\gamma \in (0, \frac{1}{2})$ in (5.53). Then the Γ -limit of F_ε defined by (5.52) on \mathcal{X}_a is*

$$F(m, \mathbf{A}) = E(m) + \frac{1}{4} \int_0^1 (D^2 V(m(t)) - \mathbf{A}(t))^2 : \mathbf{A}^{-1}(t) dt, \quad (5.57)$$

where $E(m)$ is defined by (5.50).

Γ -convergence of F_ε implies convergence of minima.

Corollary 5.4.6. *Let $(m_\varepsilon, \mathbf{A}_\varepsilon) \in \mathcal{H}_a$ be minimisers of F_ε . Then up to extracting a subsequence, $m_\varepsilon \rightarrow m$ in $\mathbf{L}^1(0, 1)$ and $\mathbf{A}_\varepsilon \rightharpoonup \mathbf{A}$ in $\mathbf{L}^1(0, 1)$ for some $m \in \mathbf{BV}(0, 1; \mathcal{C})$ and $\mathbf{A} \in \mathbf{L}_a^1(0, 1)$. Furthermore, the limit (m, \mathbf{A}) is a minimiser of F on \mathcal{X}_a .*

Remark 5.4.7. *In general convergence of minima requires both (strong) compactness and Γ -convergence; see e.g. [25]. In our case we only have weak compactness with respect to \mathbf{A}_ε for F_ε ; see Proposition 5.4.4. However, such weak convergence of \mathbf{A}_ε suffices to pass to the limit because the leading order term of the functional $F_\varepsilon(m_\varepsilon, \mathbf{A}_\varepsilon)$ is convex with respect to \mathbf{A}_ε . See the analysis of the functional (5.98) in the next section. \square*

Remark 5.4.8. *Theorem 5.4.5 shows the Γ -convergence of F_ε to F (given by (5.57)) under the assumption that \mathbf{A} is bounded away from zero, i.e. $\mathbf{A}(\cdot) \geq a \cdot \mathbf{I}_d$ for some $a > 0$. However, this assumption is unlikely to be sharp. In fact, under the weaker positivity assumption that $|\mathbf{A}(\cdot)| \geq a \cdot \mathbf{I}_d$, one can at least prove the \liminf part of the Γ -convergence of F_ε to F defined in (5.51). This is mainly because the leading order of the Green's function \mathbf{G}_ε (defined by (5.29)) depends only on $|\mathbf{A}|$; see (5.109) of Lemma (5.7.2). Although the positivity assumption is essential in our arguments for proving Theorem (5.4.5), we conjecture that the Γ -convergence result is still valid without any positivity assumption. This is to be investigated in future work.*

5.5 Conclusion

The Freidlin-Wentzell theory gives a quantitative description of the tail of the distribution of transition paths based on the theory of large deviations. It thereby leads to a natural variational definition of most likely paths in the low temperature limit, namely the minimisers of the large deviation rate functional. However, this approach exhibits some weaknesses. In particular the large deviation theory of Freidlin-Wentzell makes asymptotic statements in the limit where the noise intensity goes to zero. In practical applications the noise level

may not be small enough for these asymptotics to be valid. Furthermore, the large deviation rate functional does not exclude the possibility of the path spending large stretches of time near local maxima or saddles of the potential V . The Onsager-Machlup theory offers an alternative variational definition of most likely paths at finite temperature in terms of MAP estimators, but as shown in [188] minimisers of the Onsager-Machlup functional may be unphysical at small temperatures because the methodology fails to account for entropic effects; this can lead to transition paths which choose to make transitions through narrow energy barriers rather than (entropically favourable) wider ones with the same height, or to transition paths which (like Freidlin-Wentzell paths, although for different reasons) can spend long times at a saddle point.

We have developed an approach to the problem of identifying the most likely transition path which (like the Onsager-Machlup approach) is well-defined at finite non-vanishing temperature and yet which also recovers the correct limiting behaviour in the small temperature limit (minimisers of the Freidlin-Wentzell least action principle). Furthermore, our approach is based on finding the best Gaussian approximation with respect to Kullback-Leibler divergence, and hence captures not only the most likely path, but also the fluctuations around it. In the small temperature limit this gives the appealing interpretation that the fluctuations are defined by an OU process found from linearising the Brownian dynamics model at the minimiser of the Freidlin-Wentzell action. It is thus important to recognise that our work leads to useful characterisations of transition paths in the Brownian dynamics model, both at finite ε and in the limit $\varepsilon \rightarrow 0$. In this chapter we have concentrated exclusively on the $\varepsilon \rightarrow 0$ limit. However we now make some remarks that have bearing on both of these parameters regimes.

5.5.1 Computational Methods (Fixed ε)

Even though there is no explicit *analytic* characterisation for our notion of most likely path at finite temperature, it is possible to calculate it *numerically*. In fact, for a fixed finite temperature ε , finding the best Gaussian approximation requires minimising the functional F_ε , which involves the Kullback-Leibler divergence. In [190], a variant of the Robbins-Monro algorithm has been introduced to find best Gaussian approximations with respect to the Kullback-Leibler divergence; the numerical results in that paper demonstrate the feasibility of the minimisation, and also demonstrate that the resulting Gaussian approximation can be used to construct improved MCMC algorithms for transition paths sampling.

An important aspect of any gradient descent method to minimise an objective function is the initialisation. When the temperature ε is small but finite, the analysis in this chapter also suggests a good initialisation. Proposition 5.4.3 gives an approximate formula

for the functional F_ε :

$$F_\varepsilon = \overline{F}_\varepsilon(m_\varepsilon, \mathbf{A}_\varepsilon) + o(1),$$

where

$$\overline{F}_\varepsilon(m, \mathbf{A}) := E_\varepsilon(m) + \frac{1}{4} \int_0^1 (D^2V(m(t)) - \mathbf{A}(t))^2 : \mathbf{A}^{-1}(t) dt.$$

As a consequence, a minimiser of \overline{F}_ε provides a good approximation for the minimiser of F_ε . Approximate minimisation of the former, to obtain a good initialisation, can be carried out by make several alternations of the following two steps: first, freeze \mathbf{A} and minimise $\overline{F}_\varepsilon(m, \mathbf{A})$ as a functional of m – this can be implemented via many minimum action algorithms (see e.g. [81, 108, 120]); second, with a good approximation for m being frozen, update \mathbf{A} to be the minimiser of

$$\int_0^1 (D^2V(m(t)) - \mathbf{A}(t))^2 : \mathbf{A}^{-1}(t) dt,$$

which gives $\mathbf{A}(t) = |D^2V(m(t))|$ (see Lemma 5.7.15).

5.5.2 Interpretation of Small ε Analysis

The discussion about initialising the numerical minimisation for small ε also helps to explain our earlier assertions about the desirable structure of our minimisers when ε is small. Our main result, Theorem 5.4.5, shows that in the small temperature limit, the KL-minimisation improves on the predictions obtained by minimising the large deviation rate functional; the Γ -limit of the functional F_ε given in (5.51) consists of two parts whose minimisation decouples in the limit $\varepsilon = 0$. The first part E is closely linked with large deviation theory since it is the Γ -limit of the scaled Freidlin-Wentzell functional E_ε (Recall that E_ε arises from the Freidlin-Wentzell functional \overline{S}_T , defined in (5.3), by scaling $T = \varepsilon^{-1}$ and removing the constant $\frac{1}{2}(V(x_+) - V(x_-))$). The second part keeps track of the Ornstein-Uhlenbeck fluctuations around the optimal path and thereby captures entropic effects. Given a path m it can be minimised by choosing $\mathbf{A}(t) = |D^2V(m(t))|$. In particular, for this choice $(D^2V(m(t)) - |\mathbf{A}(t)|)^2 : |\mathbf{A}^{-1}(t)|$ is equal to zero if $D^2V(m(t))$ is positive definite (corresponding to $m(t)$ being a local minimiser of V) and strictly positive if $D^2V(m(t))$ has a negative eigenvalue (corresponding to $m(t)$ being a saddle point or a local maximum). Therefore, the Γ -limit F can be minimised explicitly as follows: first find a minimiser of E which amounts to selecting the sequence of critical points connecting x_- and x_+ that minimises the transition cost (defined by (5.47)). As shown in Section 5.4 the minimal transition cost equals to the Freidlin-Wentzell quasi-potential up to a constant and in simple cases it is given by (5.49). Then in order to minimise also the entropic part, select among

the paths which follow this sequence, those that spend no time in saddles or local maximisers. This also shows that the unphysical minimisers of the Onsager-Machlup approach (discussed in the introduction section) are removed in our approach.

5.6 Proofs of Main Results

5.6.1 Asymptotics of $F_\varepsilon^{(2)}(\mathbf{A}_\varepsilon)$

Let $\mathbf{G}_\varepsilon(t, s)$ be the Green's tensor (fundamental matrix) of the elliptic operator $(-\partial_t^2 + \mathbf{B}_\varepsilon)$ under Dirichlet boundary conditions, i.e. for any $s \in (0, 1)$,

$$\begin{aligned} (-\partial_t^2 + \varepsilon^{-2} \mathbf{A}_\varepsilon^2(\cdot) - \varepsilon^{-1} \mathbf{A}_\varepsilon'(\cdot)) \mathbf{G}_\varepsilon(\cdot, s) &= \delta(\cdot - s) \cdot \mathbf{I}_d, \\ \mathbf{G}_\varepsilon(0, s) &= \mathbf{G}_\varepsilon(1, s) = 0. \end{aligned} \quad (5.58)$$

Then by the definition of covariance operator, the expectation term in $F_\varepsilon^{(2)}(\mathbf{A}_\varepsilon)$ can be calculated in terms of the Green's tensor \mathbf{G}_ε . More precisely,

$$-\frac{\varepsilon}{4} \mathbb{E}^{\bar{\nu}_\varepsilon} \left[\int_0^1 z(t)^T \mathbf{B}_\varepsilon(t) z(t) dt \right] = -\frac{\varepsilon}{2} \int_0^1 \mathbf{B}_\varepsilon(t) : \mathbf{G}_\varepsilon(t, t) dt. \quad (5.59)$$

To simplify $F_\varepsilon^{(2)}$ we need the asymptotic estimates of \mathbf{G}_ε for small ε , which we show in the following.

5.6.1.1 Asymptotic Estimates of The Green's Tensor

For fixed $s \in (0, 1)$, the Green's tensor $\mathbf{G}_\varepsilon(\cdot, s)$ solves the linear elliptic PDE system (5.58) with variable coefficient. We want to approximate \mathbf{G}_ε by a simple Green's tensor, for which an explicit asymptotic formula is available. To do this, for any $s \in (0, 1)$, we define $\overline{\mathbf{G}}_\varepsilon(\cdot, s)$ such that

$$\begin{aligned} (-\partial_t^2 + \varepsilon^{-2} \mathbf{A}_\varepsilon^2(s)) \overline{\mathbf{G}}_\varepsilon(\cdot, s) &= \delta(\cdot - s) \cdot \mathbf{I}_d, \\ \overline{\mathbf{G}}_\varepsilon(0, s) &= \overline{\mathbf{G}}_\varepsilon(1, s) = 0. \end{aligned} \quad (5.60)$$

According to Lemma 5.7.2, when ε is small

$$\overline{\mathbf{G}}_\varepsilon(t, t) = \frac{\varepsilon}{2} (\mathbf{A}_\varepsilon^{-1}(t) + \mathbf{R}_\varepsilon(t)) \quad (5.61)$$

with $|\mathbf{R}_\varepsilon(t)| \leq C(e^{-\frac{2at}{\varepsilon}} + e^{-\frac{2a(1-t)}{\varepsilon}})$. Remember that a is the constant for which we have $\mathbf{A}_\varepsilon(t) \geq a \cdot \mathbf{I}_d$ a.e. by assumption. Furthermore, the difference $\tilde{\mathbf{R}}_\varepsilon(t, s) = \mathbf{G}_\varepsilon(t, s) - \overline{\mathbf{G}}_\varepsilon(t, s)$ admits the following bound for small ε .

Lemma 5.6.1. Let $\gamma \in (0, \frac{1}{2})$ in (5.52). Let $\{\mathbf{A}_\varepsilon\} \subset \mathbf{H}_a^1(0, 1)$ such that

$$\limsup_{\varepsilon \rightarrow 0} \varepsilon^\gamma \|\mathbf{A}_\varepsilon\|_{\mathbf{H}_a^1(0,1)}^2 < \infty.$$

Then for ε sufficiently small we have that

$$\sup_{s \in (0,1)} \|\tilde{\mathbf{R}}_\varepsilon(\cdot, s)\|_{\mathbf{L}^\infty(0,1)} \lesssim \varepsilon^{\frac{3}{2}-\gamma}, \quad (5.62)$$

and that

$$\sup_{s \in (0,1)} \|\tilde{\mathbf{R}}_\varepsilon(\cdot, s)\|_{\mathbf{L}^2(0,1)} \lesssim \varepsilon^{2-\gamma}. \quad (5.63)$$

Proof. According to (5.58) and (5.60), $\tilde{\mathbf{R}}_\varepsilon$ satisfies

$$\begin{aligned} (-\partial_t^2 + \varepsilon^{-2} \mathbf{A}_\varepsilon^2(t) - \varepsilon^{-1} \mathbf{A}'_\varepsilon(t)) \tilde{\mathbf{R}}_\varepsilon(t, s) &= \mathbf{F}_\varepsilon(t, s), \\ \tilde{\mathbf{R}}_\varepsilon(0, s) &= \tilde{\mathbf{R}}_\varepsilon(1, s) = 0, \end{aligned}$$

with

$$\mathbf{F}_\varepsilon(t, s) := (\varepsilon^{-2}(\mathbf{A}_\varepsilon^2(s) - \mathbf{A}_\varepsilon^2(t)) + \varepsilon^{-1} \mathbf{A}'_\varepsilon(t)) \overline{\mathbf{G}}_\varepsilon(t, s).$$

Let $\tilde{R}_\varepsilon^i, \overline{G}_\varepsilon^i, F_\varepsilon^i$ be the i -th column of the matrices $\tilde{\mathbf{R}}_\varepsilon, \overline{\mathbf{G}}_\varepsilon, \mathbf{F}_\varepsilon$ respectively.

$$\begin{aligned} (-\partial_t^2 + \varepsilon^{-2} \mathbf{A}_\varepsilon^2(t) - \varepsilon^{-1} \mathbf{A}'_\varepsilon(t)) \tilde{R}_\varepsilon^i(t, s) &= F_\varepsilon^i(t, s), \\ \tilde{R}_\varepsilon^i(0, s) &= \tilde{R}_\varepsilon^i(1, s) = 0. \end{aligned} \quad (5.64)$$

We only need to prove estimates (5.62) and (5.63) for each column $\tilde{R}_\varepsilon^i, i = 1, \dots, d$. To this end, we first bound the \mathbf{L}^1 -norm of the right hand side F_ε^i . In fact, by Morrey's inequality (see e.g. [90, Chapter 5]), it holds that

$$|\mathbf{A}_\varepsilon(t) - \mathbf{A}_\varepsilon(s)|_F \lesssim \|\mathbf{A}'_\varepsilon\|_{\mathbf{L}^2(0,1)} \cdot |t - s|^{\frac{1}{2}}$$

for any $t, s \in [0, 1]$. This together with (5.108) implies that

$$\begin{aligned}
& \|F_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^1(0,1)} \\
& \leq 2\varepsilon^{-2} \|\mathbf{A}_\varepsilon\|_{\mathbf{L}^\infty(0,1)} \int_0^1 |(\mathbf{A}_\varepsilon(s) - \mathbf{A}_\varepsilon(t))\overline{G}_\varepsilon^i(t, s)| dt + \varepsilon^{-1} \int_0^1 |\mathbf{A}'_\varepsilon(t)\overline{G}_\varepsilon^i(t, s)| dt \\
& \lesssim \varepsilon^{-1} \|\mathbf{A}_\varepsilon\|_{\mathbf{L}^\infty(0,1)} \cdot \|\mathbf{A}'_\varepsilon\|_{\mathbf{L}^2(0,1)} \cdot \int_0^1 |t-s|^{\frac{1}{2}} e^{-\frac{a|t-s|}{\varepsilon}} dt \\
& \quad + \|\mathbf{A}'_\varepsilon\|_{\mathbf{L}^2(0,1)} \cdot \|e^{-\frac{a|\cdot-s|}{\varepsilon}}\|_{L^2(0,1)} \\
& \lesssim \varepsilon^{\frac{1}{2}} (\|\mathbf{A}_\varepsilon\|_{\mathbf{L}^\infty(0,1)} + 1) \|\mathbf{A}'_\varepsilon\|_{\mathbf{L}^2(0,1)} \\
& \lesssim \varepsilon^{\frac{1}{2}} (\|\mathbf{A}_\varepsilon\|_{\mathbf{H}^1(0,1)} + 1) \|\mathbf{A}_\varepsilon\|_{\mathbf{H}^1(0,1)} \lesssim \varepsilon^{\frac{1}{2}-\gamma},
\end{aligned} \tag{5.65}$$

where we have used the Sobolev embedding $\mathbf{H}^1(0, 1) \hookrightarrow \mathbf{L}^\infty(0, 1)$ and the assumption that $\varepsilon^\gamma \|\mathbf{A}_\varepsilon\|_{\mathbf{H}^1(0,1)}^2 < \infty$ in the last two inequalities. Now taking the dot product of the equation (5.64) and $\tilde{R}_\varepsilon^i(\cdot, s)$ and integrating over $(0, 1)$, one obtains that

$$\begin{aligned}
|\tilde{R}_\varepsilon^i(\cdot, s)|_{\mathbf{H}^1(0,1)}^2 + \frac{a^2}{\varepsilon^2} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^2(0,1)}^2 & \leq \varepsilon^{-1} \int_0^1 |(\tilde{R}_\varepsilon^i(t, s))^T \mathbf{A}'_\varepsilon(t) \tilde{R}_\varepsilon^i(t, s)| dt \\
& \quad + \int_0^1 |\mathbf{F}_\varepsilon(t, s) \cdot \tilde{R}_\varepsilon^i(t, s)| dt.
\end{aligned} \tag{5.66}$$

We claim that the first term on the right side can be neglected when ε is small. In fact, using the Sobolev embedding $\mathbf{H}^{\frac{1}{4}}(0, 1) \hookrightarrow \mathbf{L}^4(0, 1)$ and the interpolation inequality of Lemma (5.7.7), we obtain that

$$\begin{aligned}
& \varepsilon^{-1} \int_0^1 |(\tilde{R}_\varepsilon^i(t, s))^T \mathbf{A}'_\varepsilon(t) \tilde{R}_\varepsilon^i(t, s)| dt \leq \varepsilon^{-1} \|\mathbf{A}'_\varepsilon\|_{\mathbf{L}^2(0,1)} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^4(0,1)}^2 \\
& \leq C\varepsilon^{-1} \|\mathbf{A}'_\varepsilon\|_{\mathbf{L}^2(0,1)} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{H}^{\frac{1}{4}}(0,1)}^2 \\
& \leq C\varepsilon^{-1} \|\mathbf{A}'_\varepsilon\|_{\mathbf{L}^2(0,1)} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{H}^1(0,1)}^{\frac{1}{2}} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^2(0,1)}^{\frac{3}{2}} \\
& \leq C\varepsilon^{-1-\frac{\gamma}{2}} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{H}^1(0,1)}^{\frac{1}{2}} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^2(0,1)}^{\frac{3}{2}} \\
& \leq \frac{1}{2} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{H}^1(0,1)}^2 + C\varepsilon^{-\frac{4}{3}(1+\frac{\gamma}{2})} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^2(0,1)}^2,
\end{aligned}$$

where we have used again the assumption that $\varepsilon^\gamma \|\mathbf{A}_\varepsilon\|_{\mathbf{H}^1(0,1)}^2 < \infty$ in the penultimate inequality and Young's inequality and equivalence of norm on $\mathbf{H}_0^1(0, 1)$ in the last inequality. Hence for $\gamma \in (0, \frac{1}{2})$ and ε sufficiently small, the first term on the right side of (5.66) can

be absorbed by the left hand side. This implies that

$$\begin{aligned} |\tilde{R}_\varepsilon^i(\cdot, s)|_{\mathbf{H}^1(0,1)}^2 + \frac{a^2}{\varepsilon^2} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^2(0,1)}^2 &\lesssim \int_0^1 |\mathbf{F}_\varepsilon(t, s) \cdot \tilde{R}_\varepsilon^i(t, s)| dt \\ &\leq \|\mathbf{F}_\varepsilon(\cdot, s)\|_{\mathbf{L}^1(0,1)} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^\infty(0,1)}. \end{aligned} \quad (5.67)$$

In addition, according to Lemma 5.7.8,

$$\begin{aligned} \frac{a}{\varepsilon} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^\infty(0,1)}^2 &\leq \frac{2a}{\varepsilon} |\tilde{R}_\varepsilon^i(\cdot, s)|_{\mathbf{H}^1(0,1)} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^2(0,1)} \\ &\leq |\tilde{R}_\varepsilon^i(\cdot, s)|_{\mathbf{H}^1(0,1)}^2 + \frac{a^2}{\varepsilon^2} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^2(0,1)}^2 \\ &\lesssim \|\mathbf{F}_\varepsilon(\cdot, s)\|_{\mathbf{L}^1(0,1)} \|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^\infty(0,1)}. \end{aligned}$$

Therefore we have

$$\|\tilde{R}_\varepsilon^i(\cdot, s)\|_{\mathbf{L}^\infty(0,1)} \lesssim \varepsilon \|\mathbf{F}_\varepsilon(\cdot, s)\|_{\mathbf{L}^1(0,1)}. \quad (5.68)$$

This together with (5.65) yields the estimate (5.62). Finally, the estimate (5.63) follows from (5.67), (5.68) and (5.65). \square

As a consequence of Lemma 5.6.1,

$$\mathbf{G}_\varepsilon(t, t) = \frac{\varepsilon}{2} \mathbf{A}_\varepsilon^{-1}(t) + \varepsilon \mathbf{R}_\varepsilon(t) + \tilde{\mathbf{R}}_\varepsilon(t, t) \quad (5.69)$$

where

$$|\mathbf{R}_\varepsilon(t)|_F \leq C(e^{-\frac{2at}{\varepsilon}} + e^{-\frac{2a(1-t)}{\varepsilon}}) \quad (5.70)$$

and $\tilde{\mathbf{R}}_\varepsilon$ satisfies the estimates in Lemma 5.6.1. In particular, we have

$$|\mathbf{G}_\varepsilon(t, t)|_F \leq C\varepsilon \text{ for any } t \in (0, 1). \quad (5.71)$$

Furthermore, we obtain an asymptotic formula for the expectation term in $F_\varepsilon^{(2)}(\mathbf{A}_\varepsilon)$.

Corollary 5.6.2. *Let $\gamma \in (0, \frac{1}{2})$. Let $\{\mathbf{A}_\varepsilon\} \subset \mathbf{H}_a^1(0, 1)$ such that*

$$\limsup_{\varepsilon \rightarrow 0} \varepsilon^\gamma \|\mathbf{A}_\varepsilon\|_{\mathbf{H}_a^1(0,1)}^2 < \infty.$$

Then for ε small enough we have

$$-\frac{\varepsilon}{4} \mathbb{E}^{\bar{\nu}_\varepsilon} \left[\int_0^1 z(t)^T \mathbf{B}_\varepsilon(t) z(t) dt \right] = -\frac{1}{4} \int_0^1 \text{Tr}(\mathbf{A}_\varepsilon(t)) dt + \mathcal{O}(\varepsilon^{1-2\gamma}). \quad (5.72)$$

Proof. Inserting (5.69) into the equation (5.59) and noting that $\mathbf{B}_\varepsilon = \varepsilon^{-2}\mathbf{A}_\varepsilon^2 - \varepsilon^{-1}\mathbf{A}'_\varepsilon$, we get

$$\begin{aligned} & -\frac{\varepsilon}{4}\mathbb{E}^{\overline{\nu}_\varepsilon}\left[\int_0^1 z(t)^T \mathbf{B}_\varepsilon(t) z(t) dt\right] = -\frac{1}{4}\int_0^1 \text{Tr}(\mathbf{A}_\varepsilon(t)) dt \\ & + \frac{\varepsilon}{4}\int_0^1 \text{Tr}(\mathbf{A}'_\varepsilon(t)\mathbf{A}_\varepsilon^{-1}(t)) dt - \frac{1}{2\varepsilon}\int_0^1 \text{Tr}\left((\mathbf{A}_\varepsilon^2(t) - \varepsilon\mathbf{A}'_\varepsilon(t))(\varepsilon\mathbf{R}_\varepsilon(t) + \widetilde{\mathbf{R}}_\varepsilon(t, t))\right) dt. \end{aligned} \quad (5.73)$$

Now we bound the last three terms on the right hand side. First, using the trace inequality

$$\text{Tr}(\mathbf{CD}) \lesssim |\mathbf{C}|_F |\mathbf{D}|_F, \quad (5.74)$$

which holds for any matrices \mathbf{C}, \mathbf{D} , we obtain that

$$\left|\frac{\varepsilon}{4}\int_0^1 \text{Tr}(\mathbf{A}'_\varepsilon(t)\mathbf{A}_\varepsilon^{-1}(t)) dt\right| \lesssim \varepsilon \int_0^1 |\mathbf{A}'_\varepsilon(t)|_F |\mathbf{A}_\varepsilon^{-1}(t)|_F dt \lesssim \varepsilon^{1-\frac{\gamma}{2}}. \quad (5.75)$$

In the second inequality we used the assumption that $\mathbf{A}_\varepsilon \geq a \cdot \mathbf{I}_d$ so that $\text{Tr}(\mathbf{A}_\varepsilon^{-1}) \leq d/a$ and hence $|\mathbf{A}_\varepsilon^{-1}(t)|_F \lesssim 1$. Next, applying Cauchy-Schwarz inequality to the last two terms on the right of (5.73) and using the assumptions on \mathbf{A}_ε , the inequality (5.70) and Lemma (5.6.1), we have

$$\begin{aligned} & \left|\frac{1}{2\varepsilon}\int_0^1 \text{Tr}\left((\mathbf{A}_\varepsilon^2(t) - \varepsilon\mathbf{A}'_\varepsilon(t))(\varepsilon\mathbf{R}_\varepsilon(t) + \widetilde{\mathbf{R}}_\varepsilon(t, t))\right) dt\right| \\ & \lesssim \varepsilon^{-1}\|\mathbf{A}_\varepsilon\|_{\mathbf{L}^\infty(0,1)}^2 \left(\varepsilon\|\mathbf{R}_\varepsilon\|_{\mathbf{L}^1(0,1)} + \int_0^1 |\widetilde{\mathbf{R}}_\varepsilon(t, t)| dt\right) \\ & \quad + \|\mathbf{A}'_\varepsilon\|_{\mathbf{L}^2(0,1)} \left(\varepsilon\|\mathbf{R}_\varepsilon\|_{\mathbf{L}^2(0,1)} + \left(\int_0^1 |\widetilde{\mathbf{R}}_\varepsilon(t, t)|^2 dt\right)^{\frac{1}{2}}\right) \\ & \lesssim \varepsilon^{-1-\gamma}(\varepsilon^2 + \varepsilon^{2-\gamma}) + \varepsilon^{-\frac{\gamma}{2}}(\varepsilon^{\frac{3}{2}} + \varepsilon^{2-\gamma}) \lesssim \varepsilon^{1-2\gamma}, \end{aligned} \quad (5.76)$$

where we have also used the assumption that $\gamma \in (0, \frac{1}{2})$. This finishes the proof. \square

We proceed to proving bounds for the logarithmic term appearing in $F_\varepsilon^{(2)}(\mathbf{A}_\varepsilon)$.

Lemma 5.6.3. *Let $\gamma \in (0, \frac{1}{2})$. Let $\{\mathbf{A}_\varepsilon\} \subset \mathbf{H}_a^1(0, 1)$ such that*

$$\limsup_{\varepsilon \rightarrow 0} \varepsilon^\gamma \|\mathbf{A}_\varepsilon\|_{\mathbf{H}^1(0,1)}^2 < \infty.$$

Then when ε is small enough

$$C\varepsilon \log \varepsilon \leq \frac{\varepsilon}{2} \log \left(\det \left(\int_0^1 \overline{\mathbf{M}}_\varepsilon(t) \overline{\mathbf{M}}_\varepsilon(t)^T dt \right) \right) \leq 0. \quad (5.77)$$

Proof. We first prove the non-positiveness. Since $\overline{\mathbf{M}}_\varepsilon(t) = \mathbf{M}_\varepsilon(1, t)$ where the fundamental matrix \mathbf{M}_ε satisfies (5.19) with \mathbf{A} replaced by \mathbf{A}_ε . Then the i -th column of $\overline{\mathbf{M}}_\varepsilon$, denoted by M_ε^i , satisfies

$$\partial_t M_\varepsilon^i(t, s) = -\varepsilon^{-1} \mathbf{A}_\varepsilon(t) M_\varepsilon^i(t, s), \quad M_\varepsilon^i(s, s) = e^i,$$

where e^i is the unit basis vector of \mathbf{R}^d in the i -th direction. Taking the dot product of the above equation with $M_\varepsilon^i(t, s)$ and then integrating from s to t implies that

$$|M_\varepsilon^i(t, s)|^2 = -\frac{2}{\varepsilon} \int_s^t M_\varepsilon^i(r, s)^T \mathbf{A}_\varepsilon(r) M_\varepsilon^i(r, s) dr \leq -\frac{2a}{\varepsilon} \int_s^t |M_\varepsilon^i(r, s)|^2 dr.$$

Consequently, $|M_\varepsilon^i(t, s)| \leq e^{-\frac{a(t-s)}{\varepsilon}}$ for any $0 \leq s \leq t \leq 1$. Hence each entry of $\overline{\mathbf{M}}_\varepsilon(t)$ can be bounded from above by $e^{-\frac{a(1-t)}{\varepsilon}}$. As a result, for sufficiently small ε , we have

$$\det \left(\int_0^1 \overline{\mathbf{M}}_\varepsilon(t) \overline{\mathbf{M}}_\varepsilon(t)^T dt \right) \leq C\varepsilon < 1.$$

The upper bound of (5.77) thus follows. On the other hand, applying the determinant inequality (5.116) to the matrix function $\overline{\mathbf{M}}_\varepsilon(t) \overline{\mathbf{M}}_\varepsilon(t)^T$ and the equality (5.114) yields

$$\begin{aligned} \frac{\varepsilon}{2} \log \left(\det \left(\int_0^1 \overline{\mathbf{M}}_\varepsilon(t) \overline{\mathbf{M}}_\varepsilon(t)^T dt \right) \right) &\geq \frac{\varepsilon d}{2} \log \left(\int_0^1 \det (\overline{\mathbf{M}}_\varepsilon(t))^{\frac{2}{d}} dt \right) \\ &= \frac{\varepsilon d}{2} \log \left(\int_0^1 \exp \left(-\frac{2}{\varepsilon d} \int_t^1 \text{Tr}(\mathbf{A}_\varepsilon(s)) ds \right) dt \right). \end{aligned} \quad (5.78)$$

Moreover, from the assumption that $\varepsilon^\gamma \|\mathbf{A}_\varepsilon\|_{\mathbf{H}^1(0,1)}^2 < \infty$ and the fact that $\mathbf{H}^1(0,1)$ is embedded into $\mathbf{L}^\infty(0,1)$, we obtain that

$$\int_t^1 \text{Tr}(\mathbf{A}_\varepsilon(s)) ds \leq (1-t) \|\mathbf{A}_\varepsilon\|_{\mathbf{L}^\infty(0,1)} \leq C\varepsilon^{-\frac{\gamma}{2}} (1-t).$$

Combining this with (5.78) gives

$$\begin{aligned} \frac{\varepsilon}{2} \log \left(\det \left(\int_0^1 \overline{\mathbf{M}}_\varepsilon(t) \overline{\mathbf{M}}_\varepsilon(t)^T dt \right) \right) &\geq \frac{\varepsilon d}{2} \log \left(\int_0^1 \exp \left(-\frac{2C}{\varepsilon^{1+\frac{\gamma}{2}}d} (1-t) \right) dt \right) \\ &= \frac{\varepsilon d}{2} \log \left(\frac{\varepsilon^{1+\frac{\gamma}{2}}d}{2C} \left(1 - e^{-\frac{2C}{\varepsilon^{1+\frac{\gamma}{2}}d}} \right) \right) \\ &\geq C\varepsilon \log \varepsilon \end{aligned} \quad (5.79)$$

for sufficiently small ε . This completes the proof. \square

Recall that the definition of $F_\varepsilon^{(2)}$ in (5.54). Then the following proposition, containing the asymptotic expression for $F_\varepsilon^{(2)}(\mathbf{A}_\varepsilon)$, is a direct consequence of Corollary 5.6.2 and Lemma (5.6.3).

Proposition 5.6.4. *Let $\{\mathbf{A}_\varepsilon\} \subset \mathbf{H}_a^1(0, 1)$ such that $\limsup_{\varepsilon \rightarrow 0} \varepsilon^\gamma \|\mathbf{A}_\varepsilon\|_{\mathbf{H}^1(0,1)}^2 < \infty$ with $\gamma \in (0, \frac{1}{2})$. Then it holds that*

$$F_\varepsilon^{(2)}(\mathbf{A}_\varepsilon) = \frac{1}{4} \int_0^1 \text{Tr}(\mathbf{A}_\varepsilon(t)) dt + \mathcal{O}(\varepsilon^{1-\gamma}), \quad (5.80)$$

when ε is small enough.

5.6.2 Asymptotics of $F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon)$

In this subsection, we seek an asymptotic expression for $F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon)$ when it is uniformly bounded with respect to ε . We start by showing that the boundedness of $F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon)$ implies the boundedness of $\|m_\varepsilon\|_{\mathbf{L}^\infty(0,1)}$.

Lemma 5.6.5. *Assume that $(m_\varepsilon, \mathbf{A}_\varepsilon) \in \mathcal{H}$ and that $\limsup_{\varepsilon \rightarrow 0} F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon) < \infty$. Then we have $\limsup_{\varepsilon \rightarrow 0} \|m_\varepsilon\|_{\mathbf{L}^\infty(0,1)} < \infty$.*

Proof. Recalling that $\Psi_\varepsilon(x) = \frac{1}{2}|\nabla V(x)|^2 - \varepsilon \Delta V(x)$ and that $\nu_\varepsilon = N(m_\varepsilon, \Sigma_\varepsilon)$, we can rewrite $F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon)$ as

$$\begin{aligned} F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon) &= \frac{\varepsilon}{4} \int_0^1 |m'_\varepsilon(t)|^2 dt + \frac{1}{2\varepsilon} \mathbb{E}^{\overline{\nu}_\varepsilon} \left[\int_0^1 \Psi_\varepsilon(z(t) + m_\varepsilon(t)) dt \right] \\ &= F_\varepsilon^{(3)}(m_\varepsilon, \mathbf{A}_\varepsilon) + F_\varepsilon^{(4)}(m_\varepsilon, \mathbf{A}_\varepsilon) \end{aligned}$$

where

$$F_\varepsilon^{(3)}(m_\varepsilon, \mathbf{A}_\varepsilon) := \frac{\varepsilon}{4} \int_0^1 |m'_\varepsilon(t)|^2 dt + \frac{1}{8\varepsilon} \int_0^1 \mathbb{E}^{\overline{\nu}_\varepsilon} [|\nabla V(z(t) + m_\varepsilon(t))|^2] dt$$

and

$$\begin{aligned} F_\varepsilon^{(4)}(m_\varepsilon, \mathbf{A}_\varepsilon) &:= \frac{1}{8\varepsilon} \int_0^1 \mathbb{E}^{\bar{\nu}_\varepsilon} [|\nabla V(z(t) + m_\varepsilon(t))|^2 - 4\varepsilon \Delta V(z(t) + m_\varepsilon(t))] dt \\ &= \frac{1}{8\varepsilon} \int_0^1 \mathbb{E}^{\nu_\varepsilon} [|\nabla V(x(t))|^2 - 4\varepsilon \Delta V(x(t))] dt. \end{aligned}$$

First, from (5.16) of Remark 5.2.2 we can obtain immediately that

$$\liminf_{\varepsilon \rightarrow 0} F_\varepsilon^{(4)}(m_\varepsilon, \mathbf{A}_\varepsilon) > -\infty.$$

This together with the assumption that $\limsup_{\varepsilon \rightarrow 0} F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon) < \infty$ implies

$$\limsup_{\varepsilon \rightarrow 0} F_\varepsilon^{(3)}(m_\varepsilon, \mathbf{A}_\varepsilon) < \infty.$$

We now show that this implies the uniformly boundedness of $\|m_\varepsilon\|_{\mathbf{L}^\infty(0,1)}$.

We prove a lower bound for $F_\varepsilon^{(3)}(m_\varepsilon, \mathbf{A}_\varepsilon)$. Given any $R > 0$, define $T_\varepsilon^R := \{t \in (0, 1) : |m_\varepsilon(t)| > R\}$ which is an open set on $(0, 1)$. By restricting the second integral and expectation over a smaller set, we have

$$F_\varepsilon^{(3)}(m_\varepsilon, \mathbf{A}_\varepsilon) \geq \frac{\varepsilon}{4} \int_0^1 |m'_\varepsilon(t)|^2 dt + \frac{1}{8\varepsilon} \int_{T_\varepsilon^R} \mathbb{E}^{\bar{\nu}_\varepsilon} [|\nabla V(m_\varepsilon(t) + z(t))|^2 \mathbf{1}_{\{|z(t)| \leq \varepsilon^{1/4}\}}] dt. \quad (5.81)$$

Consider (t, ω) such that $|m_\varepsilon(t)| > R$ and $|z(t, \omega)| \leq \varepsilon^{1/4}$. If $\varepsilon > 0$ is small enough to satisfy $\varepsilon^{1/4} < R/2$, then

$$|m_\varepsilon(t) + z(t, \omega)| \geq |m_\varepsilon(t)| - |z(t, \omega)| \geq |m_\varepsilon(t)|/2.$$

Combining this with the monotonicity condition (A-6) yields that

$$\begin{aligned} &\frac{1}{8\varepsilon} \int_{T_\varepsilon^R} \mathbb{E}^{\bar{\nu}_\varepsilon} [|\nabla V(m_\varepsilon(t) + z(t))|^2 \mathbf{1}_{\{|z(t)| \leq \varepsilon^{1/4}\}}] dt \\ &\geq \frac{1}{8\varepsilon} \int_{T_\varepsilon^R} |\nabla V(m_\varepsilon(t)/2)|^2 \bar{\nu}_\varepsilon \left(\{|z(t)| \leq \varepsilon^{1/4}\} \right) dt \geq \frac{1}{16\varepsilon} \int_{T_\varepsilon^R} |\nabla V(m_\varepsilon(t)/2)|^2 dt \end{aligned} \quad (5.82)$$

when $\varepsilon > 0$ is small enough. We have used the fact that $\bar{\nu}_\varepsilon \left(\{|z(t)| \leq \varepsilon^{1/4}\} \right) \geq 1/2$ for any $t \in (0, 1)$ and small ε . This is because $z(t)$ is a centred Gaussian random variable with covariance $2\mathbf{G}_\varepsilon(t, t)$ (see (5.28)). In addition, we know from (5.71) that $|\mathbf{G}_\varepsilon(t, t)|_F \leq C\varepsilon$ for any $t \in (0, 1)$ and hence $\bar{\nu}_\varepsilon \left(\{|z(t)| \leq \varepsilon^{1/4}\} \right) \rightarrow 1$ when $\varepsilon \rightarrow 0$. Let $\tilde{m}_\varepsilon = m_\varepsilon/2$. From

(5.81), (5.82) and the uniform boundedness of $F_\varepsilon^{(3)}(m_\varepsilon, \mathbf{A}_\varepsilon)$ we obtain

$$\limsup_{\varepsilon \rightarrow 0} \varepsilon \int_{T_\varepsilon^R} |\tilde{m}'_\varepsilon(t)|^2 dt + \frac{1}{16\varepsilon} \int_{T_\varepsilon^R} |\nabla V(\tilde{m}_\varepsilon(t))|^2 dt < \infty.$$

Then application of the elementary inequality $2ab \leq a^2 + b^2$ yields

$$\limsup_{\varepsilon \rightarrow 0} \int_{T_\varepsilon^R} |\tilde{m}'_\varepsilon(t)| |\nabla V(\tilde{m}_\varepsilon(t))| dt < \infty.$$

Choosing a sufficiently large R and by the coercivity condition (A-3), we have

$$\limsup_{\varepsilon \rightarrow 0} \int_{T_\varepsilon^R} |\tilde{m}'_\varepsilon(t)| < \infty. \quad (5.83)$$

Now we conclude the uniform boundedness of $\|m_\varepsilon\|_{L^\infty(0,1)}$ by applying the same argument used for proving Theorem 1.2 in [149]. Specifically, since m_ε is continuous on $(0, 1)$, T_ε^R is open on $(0, 1)$ and we can write $T_\varepsilon^R = \cup_{i=1}^\infty (a_\varepsilon^i, b_\varepsilon^i)$. Suppose that T_ε^R is empty, then $|m_\varepsilon(t)| \leq R$ for all $t \in (0, 1)$. Otherwise, consider $\tilde{m}_\varepsilon(t)$ with $t \in (a_\varepsilon^i, b_\varepsilon^i)$. Obviously at least one of the end points of the subinterval, say a_ε^i is not an endpoint of $(0, 1)$. Then we should have $|m_\varepsilon(a_\varepsilon^i)| = R$ and hence $|\tilde{m}_\varepsilon(a_\varepsilon^i)| = 2R$. Thus we get from the fundamental theorem of calculus that

$$\begin{aligned} \limsup_{\varepsilon \rightarrow 0} \sup_{t \in (a_\varepsilon^i, b_\varepsilon^i)} |\tilde{m}_\varepsilon(t)| &\leq \limsup_{\varepsilon \rightarrow 0} \left(|\tilde{m}_\varepsilon(a_\varepsilon^i)| + \sup_{t \in (a_\varepsilon^i, b_\varepsilon^i)} \left| \int_{a_\varepsilon^i}^t \tilde{m}_\varepsilon(s) ds \right| \right) \\ &\leq 2R + \limsup_{\varepsilon \rightarrow 0} \int_{T_\varepsilon^R} |\tilde{m}'_\varepsilon(t)| < \infty \end{aligned}$$

where the last inequality follows from (5.83). Therefore $\limsup_{\varepsilon \rightarrow 0} \|m_\varepsilon\|_{L^\infty(0,1)} < \infty$. \square

Next, the expectation term of $F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon)$ can be simplified under the condition that $\|m_\varepsilon\|_{L^\infty(0,1)}$ is uniformly bounded.

Lemma 5.6.6. *Let $(m_\varepsilon, \mathbf{A}_\varepsilon) \in \mathcal{H}$. Assume that $\limsup_{\varepsilon \rightarrow 0} \varepsilon^\gamma \|\mathbf{A}_\varepsilon\|_{\mathbf{H}^1(0,1)}^2 < \infty$ with $\gamma \in (0, \frac{1}{2})$ and that $\limsup_{\varepsilon \rightarrow 0} \|m_\varepsilon\|_{L^\infty(0,1)} < \infty$. Then for $\varepsilon > 0$ small enough we have*

$$\begin{aligned} F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon) &= E_\varepsilon(m_\varepsilon) - \frac{1}{2} \int_0^1 \Delta V(m_\varepsilon(t)) dt \\ &\quad + \frac{1}{4} \int_0^1 (D^2 V(m_\varepsilon(t))^2 + D^3 V(m_\varepsilon(t)) \cdot \nabla V(m_\varepsilon(t))) : \mathbf{A}_\varepsilon^{-1}(t) dt + \mathcal{O}(\varepsilon^{\frac{1}{2}}). \end{aligned}$$

Proof. Remember that

$$F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon) = \frac{\varepsilon}{4} \int_0^1 |m'(t)|^2 dt + \frac{1}{2\varepsilon} \mathbb{E}^{\bar{\nu}_\varepsilon} \left[\int_0^1 \Psi_\varepsilon(m_\varepsilon(t) + z_\varepsilon(t)) dt \right].$$

To evaluate the expectation term of $F_\varepsilon^{(1)}(m_\varepsilon, \mathbf{A}_\varepsilon)$, we use the following multi-variable Taylor's formula for Ψ_ε :

$$\Psi_\varepsilon(x(t)) = \Psi_\varepsilon(m_\varepsilon(t)) + \nabla \Psi_\varepsilon(m_\varepsilon(t)) \cdot z_\varepsilon(t) + \frac{1}{2} z_\varepsilon(t)^T D^2 \Psi_\varepsilon(m_\varepsilon(t)) z_\varepsilon(t) + r_\varepsilon(t),$$

where the reminder term r_ε is given in integral form by

$$r_\varepsilon(t) = \sum_{|\alpha|=3} \frac{z_\varepsilon^\alpha(t)}{\alpha!} \int_0^1 \partial^\alpha \Psi_\varepsilon(m_\varepsilon(t) + \xi z_\varepsilon(t)) (1-\xi)^3 d\xi.$$

Here $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_d)$ is a multi-index and we use the notational convention $x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \dots x_d^{\alpha_d}$ and $\partial^\alpha f = \partial_1^{\alpha_1} \partial_2^{\alpha_2} \dots \partial_d^{\alpha_d} f$. Then using again the fact that $z_\varepsilon(t) \sim N(0, 2\mathbf{G}_\varepsilon(t, t))$, we obtain that

$$\begin{aligned} & \frac{1}{2\varepsilon} \mathbb{E}^{\bar{\nu}_\varepsilon} \left[\int_0^1 \Psi_\varepsilon(m_\varepsilon(t) + z_\varepsilon(t)) dt \right] \\ &= \frac{1}{2\varepsilon} \int_0^1 \Psi_\varepsilon(m_\varepsilon(t)) dt + \frac{1}{2\varepsilon} \int_0^1 D^2 \Psi_\varepsilon(m_\varepsilon(t)) : \mathbf{G}_\varepsilon(t, t) dt + \frac{1}{2\varepsilon} \int_0^1 \mathbb{E}^{\bar{\nu}_\varepsilon} [r_\varepsilon(t)] dt. \end{aligned} \quad (5.84)$$

Recalling that $\Psi_\varepsilon(x) = \frac{1}{2} |\nabla V(x)|^2 - \varepsilon \Delta V(x)$, we have

$$D^2 \Psi_\varepsilon(x) = (D^2 V(x))^2 + D^3 V(x) \cdot \nabla V(x) - \varepsilon D^2 (\Delta V(x)).$$

From this equation, the expression (5.69) for $\mathbf{G}_\varepsilon(t, t)$ and the uniform boundedness of $\|m_\varepsilon\|_{\mathbf{L}^\infty(0,1)}$, the second term on the right side of (5.84) becomes

$$\begin{aligned} & \frac{1}{2\varepsilon} \int_0^1 D^2 \Psi_\varepsilon(m_\varepsilon(t)) : \mathbf{G}_\varepsilon(t, t) dt \\ &= \frac{1}{4} \int_0^1 \left((D^2 V(m_\varepsilon(t)))^2 + D^3 V(m_\varepsilon(t)) \cdot \nabla V(m_\varepsilon(t)) \right) : \mathbf{A}_\varepsilon^{-1}(t) dt + \mathcal{O}(\varepsilon). \end{aligned} \quad (5.85)$$

Next we claim that the integral of the last term on the right hand side of (5.84) is of order $\mathcal{O}(\varepsilon^{\frac{3}{2}})$. Indeed, from the assumption (5.13) and the fact that $z_\varepsilon(t) = N(0, 2\mathbf{G}_\varepsilon(t, t))$ with

$\mathbf{G}_\varepsilon(t, t)$ satisfying the estimate (5.71), we have

$$\begin{aligned}
\mathbb{E}^{\nu_\varepsilon}[r_\varepsilon(t)] &\leq \sum_{|\alpha|=3} \frac{1}{\alpha!} \max_{\xi \in [0,1]} \left\{ \mathbb{E}^{\nu_\varepsilon} \left[|z_\varepsilon(t)|^3 \partial_\alpha \Psi_\varepsilon(m_\varepsilon(t) + \xi z_\varepsilon(t)) \right] \right\} \\
&\leq \frac{C_1}{\sqrt{(4\pi)^d \det(2\mathbf{G}_\varepsilon(t, t))}} \max_{\xi \in [0,1]} \left\{ \int_{\mathbf{R}^d} |x|^3 e^{C_2|m_\varepsilon(t)+\xi x|^\alpha} \cdot e^{-\frac{1}{4}x^T \mathbf{G}_\varepsilon(t,t)^{-1}x} dx \right\} \\
&\leq \frac{C_1}{\sqrt{(4\pi)^d \det(\mathbf{G}_\varepsilon(t, t))}} e^{2C_2\|m_\varepsilon\|_{\mathbf{L}^\infty(0,1)}^2} \int_{\mathbf{R}^d} e^{2C_2|x|^\alpha} |x|^3 e^{-\frac{1}{4}x^T \mathbf{G}_\varepsilon(t,t)^{-1}x} dx \\
&\leq \frac{C_2}{\sqrt{(4\pi)^d}} |\mathbf{G}_\varepsilon(t, t)|_F^{\frac{3}{2}} \cdot e^{2C_2\|m_\varepsilon\|_{\mathbf{L}^\infty(0,1)}^2} \cdot \int_{\mathbf{R}^d} |x|^3 e^{-\frac{|x|^2}{4}} dx \leq C\varepsilon^{\frac{3}{2}}.
\end{aligned} \tag{5.86}$$

when ε is small enough. Notice that in last two inequalities of above we used the fact that $\alpha \in [0, 2)$ and that $|\mathbf{G}_\varepsilon(t, t)|_F \leq C\varepsilon$ so that $e^{2C_2|x|^\alpha}$ can be absorbed by $e^{\frac{1}{4}x^T \mathbf{G}_\varepsilon(t,t)^{-1}x}$ for large x . Then the desired result follows from (5.84), (5.85) and (5.86). \square

5.6.3 Proof of Main Results

Proof of Proposition 5.4.3. The proposition follows directly from the definition of F_ε , Proposition 5.6.4, Lemma 5.6.6 and the following equalities

$$\begin{aligned}
&-2\Delta V + (D^2V)^2 : \mathbf{A}^{-1} + \text{Tr}(\mathbf{A}) \\
&= -2\text{Tr}(D^2V) + \text{Tr}((D^2V)^2 \mathbf{A}^{-1}) + \text{Tr}(\mathbf{A}^2 \mathbf{A}^{-1}) \\
&= -\text{Tr}((\mathbf{A} D^2V \mathbf{A}^{-1}) - \text{Tr}(\mathbf{A}^{-1} D^2V \mathbf{A}) + \text{Tr}((D^2V)^2 \mathbf{A}^{-1}) + \text{Tr}(\mathbf{A}^2 \mathbf{A}^{-1}) \\
&= (D^2V - \mathbf{A})^2 : \mathbf{A}^{-1},
\end{aligned} \tag{5.87}$$

which are valid for any $V \in C^2(\mathbf{R}^d)$ and any positive definite matrix \mathbf{A} . \square

The following lemma shows that $\varepsilon \log(Z_{\mu,\varepsilon})$ is bounded from above.

Lemma 5.6.7. *There exists $C > 0$ depending only on the potential V such that the following holds:*

$$\limsup_{\varepsilon \rightarrow 0} \varepsilon \log(Z_{\mu,\varepsilon}) \leq C. \tag{5.88}$$

Proof. Recall that

$$Z_{\mu,\varepsilon} = \mathbb{E}^{\mu_0} \left[\exp \left(-\frac{1}{2\varepsilon^2} \int_0^1 |\nabla V(x(t))|^2 - \varepsilon \Delta V(x(t)) dt \right) \right].$$

From (5.16) of Remark 5.2.2,

$$Z_{\mu,\varepsilon} \leq \exp \left(\frac{C}{\varepsilon} \right)$$

with some $C > 0$. This proves (5.88). \square

Proof of Proposition 5.4.4. Assume that $\limsup_n F_{\varepsilon_n}(m_n, \mathbf{A}_n) < \infty$. Since the Kullback-Leibler divergence $D_{\text{KL}}(\nu_{\varepsilon_n} \parallel \mu_{\varepsilon_n})$ is always non-negative, it follows from (5.40) and Lemma 5.6.7 that

$$\liminf_{n \rightarrow \infty} \varepsilon_n \tilde{D}_{\text{KL}}(\nu_{\varepsilon_n} \parallel \mu_{\varepsilon_n}) \geq -C \quad (5.89)$$

for some $C > 0$. This together with the assumption that $\limsup_n F_{\varepsilon_n}(m_n, \mathbf{A}_n) < \infty$ implies that $\limsup_n \varepsilon_n^\gamma \|\mathbf{A}_n\|_{\mathbf{H}^1(0,1)}^2 < \infty$. Then from Proposition 5.6.4 and noting that $\mathbf{A}(\cdot) - a \cdot \mathbf{I}_d \geq 0$, we obtain

$$\limsup_n F_{\varepsilon_n}^{(2)}(\mathbf{A}_n) \geq \limsup_n \frac{1}{4} \int_0^1 \text{Tr}(\mathbf{A}_n(t)) dt \geq \frac{da}{4}.$$

Hence we have $\limsup_n F_{\varepsilon_n}^{(1)}(m_n, \mathbf{A}_n) < \infty$. Then Lemma 5.6.5 implies that

$$\limsup_n \|m_n\|_{\mathbf{L}^\infty(0,1)} < \infty.$$

Hence as a consequence of Lemma 5.6.6,

$$\begin{aligned} F_{\varepsilon_n}(m_n, \mathbf{A}_n) &= E_{\varepsilon_n}(m_n) + \frac{1}{4} \int_0^1 (D^2 V(m_n(t)) - \mathbf{A}_n(t))^2 : \mathbf{A}_n^{-1}(t) dt \\ &\quad + \int_0^1 (D^3 V(m_n(t)) \cdot \nabla V(m_n(t))) : \mathbf{A}_n^{-1}(t) dt + \varepsilon_n^\gamma \|\mathbf{A}_n\|_{\mathbf{H}^1(0,1)}^2 + \mathcal{O}(\varepsilon_n^{\frac{1}{2}}). \end{aligned} \quad (5.90)$$

The second term on the right side of above is nonnegative. In addition, owing to the trace inequality (5.74) and the fact that $\mathbf{A}_n \geq a \cdot \mathbf{I}_d$,

$$\begin{aligned} &\limsup_n \left| \frac{1}{4} \int_0^1 D^3 V(m_n(t)) \cdot \nabla V(m_n(t)) : \mathbf{A}_n^{-1}(t) dt \right| \\ &\leq \limsup_n \int_0^1 \left| (D^3 V(m_n(t)) \cdot \nabla V(m_n(t)))^2 \right|_F |\mathbf{A}_n^{-1}(t)|_F dt < \infty. \end{aligned} \quad (5.91)$$

This implies from (5.90) that $\limsup_n E_{\varepsilon_n}(m_n) < \infty$. By the compactness result of Lemma 5.4.1, there exists $m \in \mathbf{BV}(0, 1; \mathcal{E})$ and a subsequence m_{n_k} such that $m_{n_k} \rightarrow m$ in $\mathbf{L}^1(0, 1)$. Moreover, we know from the above reasoning that

$$\limsup_n \frac{1}{4} \int_0^1 (D^2 V(m_n(t)) - \mathbf{A}_n(t))^2 : \mathbf{A}_n^{-1}(t) dt < \infty \quad (5.92)$$

from which we can conclude that $\sup_n \|\mathbf{A}_n\|_{\mathbf{L}^1(0,1)} < \infty$. Indeed,

$$\begin{aligned} & \int_0^1 (D^2V(m_n(t)) - \mathbf{A}_n(t))^2 : \mathbf{A}_n^{-1}(t) dt \\ &= \int_0^1 \text{Tr} \left((D^2V(m_n(t)))^2 \mathbf{A}_n^{-1}(t) \right) dt - 2 \int_0^1 \text{Tr} (D^2V(m_n(t))) dt + \int_0^1 \text{Tr}(\mathbf{A}_n(t)) dt. \end{aligned} \quad (5.93)$$

The first term on the right of above is non-negative. The second term is clearly bounded since $\|m_n\|_{\mathbf{L}^\infty(0,1)}$ is uniformly bounded. Hence $\sup_n \|\mathbf{A}_n\|_{\mathbf{L}^1(0,1)} < \infty$ follows from (5.92), (5.93) and the inequality $|\mathbf{A}|_F \leq \text{Tr}(\mathbf{A})$ which holds for any positive definite matrix \mathbf{A} . \square

The proof of Γ -limit of F_ε is presented in what follows.

Proof of Theorem 5.4.5. We start by proving the liminf inequality, i.e.

$$F(m, \mathbf{A}) \leq \liminf_{\varepsilon \rightarrow 0} F_\varepsilon(m_\varepsilon, \mathbf{A}_\varepsilon)$$

for any sequence $\{(m_\varepsilon, \mathbf{A}_\varepsilon)\}$ such that $(m_\varepsilon, \mathbf{A}_\varepsilon) \rightarrow (m, \mathbf{A})$ in \mathcal{X} , or equivalently $m_\varepsilon \rightarrow m$ and $\mathbf{A}_\varepsilon \rightharpoonup \mathbf{A}$ in $\mathbf{L}^1(0,1)$. We may assume that $\liminf_{\varepsilon \rightarrow 0} F_\varepsilon(m_\varepsilon, \mathbf{A}_\varepsilon) < \infty$ since otherwise there is nothing to prove. Then by the same argument used in the proof of Proposition 5.4.4, one can get $\limsup_{\varepsilon \rightarrow 0} \varepsilon^\gamma \|\mathbf{A}_\varepsilon\|_{\mathbf{H}^1(0,1)}^2 < \infty$. Let $\{\varepsilon_k\}$ be a sequence such that $\varepsilon_k \rightarrow 0$ as $k \rightarrow \infty$ and $\lim_{k \rightarrow \infty} F_{\varepsilon_k}(m_{\varepsilon_k}, \mathbf{A}_{\varepsilon_k}) = \liminf_{\varepsilon \rightarrow 0} F_\varepsilon(m_\varepsilon, \mathbf{A}_\varepsilon) < \infty$. Since $\mathbf{A}_{\varepsilon_k} \geq a \cdot \mathbf{I}_d$ a.e., it follows from $\mathbf{A}_{\varepsilon_k} \rightharpoonup \mathbf{A}$ and Mazur's lemma (Lemma 5.7.16) that the limit $\mathbf{A} \geq a \cdot \mathbf{I}_d$ a.e. According to Proposition 5.6.4 and $\mathbf{A}_{\varepsilon_k} \rightharpoonup \mathbf{A}$ in $\mathbf{L}^1(0,1)$, it holds that

$$\lim_{k \rightarrow \infty} F_{\varepsilon_k}^{(2)}(\mathbf{A}_{\varepsilon_k}) = \frac{1}{4} \int_0^1 \text{Tr}(\mathbf{A}(t)) dt \geq \frac{da}{4}.$$

Then it follows that $\lim_{k \rightarrow \infty} F_{\varepsilon_k}^{(1)}(m_{\varepsilon_k}, \mathbf{A}_{\varepsilon_k}) < \infty$. From Lemma 5.6.5 we obtain that $\|m_{\varepsilon_k}\|_{\mathbf{L}^\infty(0,1)}$ is uniformly bounded. Hence as a consequence of Lemma 5.6.6,

$$\begin{aligned} F_{\varepsilon_k}^{(1)}(m_{\varepsilon_k}, \mathbf{A}_{\varepsilon_k}) &= E_\varepsilon(m_{\varepsilon_k}) - \frac{1}{2} \int_0^1 \Delta V(m_{\varepsilon_k}(t)) dt \\ &+ \frac{1}{4} \int_0^1 (D^2V(m_{\varepsilon_k}(t))^2 + D^3V(m_{\varepsilon_k}(t)) \cdot \nabla V(m_{\varepsilon_k}(t))) : \mathbf{A}_{\varepsilon_k}^{-1}(t) dt + O(\varepsilon_k^{\frac{1}{2}}). \end{aligned}$$

In addition, it follows from the uniform boundedness of $\|m_{\varepsilon_k}\|_{\mathbf{L}^\infty(0,1)}$ and $\mathbf{A}_{\varepsilon_k} \rightharpoonup \mathbf{A}$ in

$\mathbf{L}^1(0, 1)$ that

$$\limsup_{k \rightarrow \infty} \left\{ \left| -\frac{1}{2} \int_0^1 \Delta V(m_{\varepsilon_k}(t)) dt \right. \right. \\ \left. \left. + \frac{1}{4} \int_0^1 (D^2 V(m_{\varepsilon_k}(t))^2 + D^3 V(m_{\varepsilon_k}(t)) \cdot \nabla V(m_{\varepsilon_k}(t))) : \mathbf{A}_{\varepsilon_k}^{-1}(t) dt \right| \right\} < \infty.$$

This in turn implies that $\limsup_{k \rightarrow \infty} E_{\varepsilon_k}(m_{\varepsilon_k}) < \infty$. By the compactness result in Lemma 5.4.1, we have $m \in \mathbf{BV}((0, 1); \mathcal{E})$. Furthermore, by passing to a subsequence, we may assume further that $m_{\varepsilon_k} \rightarrow m$ a.e. on $[0, 1]$. Since m takes value in \mathcal{E} a.e. on $[0, 1]$, we use the definition of $D^3 V$ and the dominated convergence theorem to conclude that

$$\int_0^1 (D^3 V(m_{\varepsilon_k}(t)) \cdot \nabla V(m_{\varepsilon_k}(t))) : \mathbf{A}_{\varepsilon_k}^{-1}(t) dt \rightarrow 0. \quad (5.94)$$

In fact, similar to (5.91), we have

$$\int_0^1 \left| (D^3 V(m_{\varepsilon_k}(t)) \cdot \nabla V(m_{\varepsilon_k}(t))) : \mathbf{A}_{\varepsilon_k}^{-1}(t) \right| dt < \infty.$$

In addition, since $\nabla V(m_{\varepsilon_k}(t)) \rightarrow 0$ a.e. on $[0, 1]$ and $\mathbf{A}_{\varepsilon_k} \geq a \cdot \mathbf{I}_d$, we have

$$\begin{aligned} & \left| (D^3 V(m_{\varepsilon_k}(t)) \cdot \nabla V(m_{\varepsilon_k}(t))) : \mathbf{A}_{\varepsilon_k}^{-1}(t) \right| \\ & \leq \left| D^3 V(m_{\varepsilon_k}(t)) \cdot \nabla V(m_{\varepsilon_k}(t)) \right|_F \left| \mathbf{A}_{\varepsilon_k}^{-1}(t) \right|_F \rightarrow 0 \end{aligned} \quad (5.95)$$

a.e. on $[0, 1]$. This proves (5.94). Now we claim that

$$\begin{aligned} & \int_0^1 (D^2 V(m(t)) - \mathbf{A}(t))^2 : \mathbf{A}^{-1}(t) dt \\ & \leq \liminf_{k \rightarrow \infty} \int_0^1 (D^2 V(m_{\varepsilon_k}(t)) - \mathbf{A}_{\varepsilon_k}(t))^2 : \mathbf{A}_{\varepsilon_k}^{-1}(t) dt \end{aligned} \quad (5.96)$$

when $m_{\varepsilon_k} \rightarrow m$ in $\mathbf{L}^1(0, 1)$ with $m(\cdot) \in \mathcal{E}$ a.e. and $\mathbf{A}_{\varepsilon_k} \rightharpoonup \mathbf{A}$ in $\mathbf{L}^1(0, 1)$. In fact, the weak convergence $\mathbf{A}_{\varepsilon_k} \rightharpoonup \mathbf{A}$ in $\mathbf{L}^1(0, 1)$ directly implies that

$$\int_0^1 \mathbf{A}_{\varepsilon_k}^2(t) : \mathbf{A}_{\varepsilon_k}^{-1}(t) - \mathbf{A}^2(t) : \mathbf{A}^{-1}(t) dt = \int_0^1 \text{Tr}(\mathbf{A}_{\varepsilon_k}(t) - \mathbf{A}(t)) dt \rightarrow 0.$$

In addition, thanks to the uniform boundedness of $\|m_{\varepsilon_k}\|_{\mathbf{L}^\infty(0, 1)}$ and the strong convergence

$m_{\varepsilon_k} \rightarrow m$ in $\mathbf{L}^1(0, 1)$, we obtain from the dominated convergence that

$$\begin{aligned} & \int_0^1 (D^2V(m_{\varepsilon_k}(t))\mathbf{A}_{\varepsilon_k}(t) + \mathbf{A}_{\varepsilon_k}(t)D^2V(m_{\varepsilon_k}(t))) : \mathbf{A}_{\varepsilon_k}^{-1}(t)dt \\ & - \int_0^1 (D^2V(m(t))\mathbf{A}(t) + \mathbf{A}(t)D^2V(m(t))) : \mathbf{A}^{-1}(t)dt \\ & = 2 \int_0^1 \text{Tr}(D^2V(m_{\varepsilon_k}(t)) - D^2V(m(t)))dt \rightarrow 0. \end{aligned}$$

Therefore to prove (5.96), we need to check

$$\int_0^1 D^2(m(t))^2 : \mathbf{A}^{-1}(t)dt \leq \liminf_{k \rightarrow \infty} \int_0^1 D^2V(m_{\varepsilon_k}(t))^2 : \mathbf{A}_{\varepsilon_k}^{-1}(t)dt.$$

From the equality

$$\begin{aligned} & \int_0^1 D^2V(m_{\varepsilon_k}(t))^2 : \mathbf{A}_{\varepsilon_k}^{-1}(t)dt = \int_0^1 D^2V(m(t))^2 : \mathbf{A}_{\varepsilon_k}^{-1}(t)dt \\ & + \int_0^1 (D^2V(m_{\varepsilon_k}(t))^2 - D^2V(m(t))^2) : \mathbf{A}_{\varepsilon_k}^{-1}(t)dt, \end{aligned}$$

the assumption that $m_{\varepsilon_k} \rightarrow m$ in $\mathbf{L}^1(0, 1)$ and that $\mathbf{A}_{\varepsilon_k}^{-1} \geq a \cdot \mathbf{I}_d$, it suffices to show

$$\int_0^1 D^2(m(t))^2 : \mathbf{A}^{-1}(t)dt \leq \liminf_{k \rightarrow \infty} \int_0^1 D^2V(m(t))^2 : \mathbf{A}_{\varepsilon_k}^{-1}(t)dt =: \theta. \quad (5.97)$$

To that end, let $\mathbf{B}(\cdot) := D^2V(m(\cdot))^2$. Noting that $m(\cdot) \in \mathcal{E}$ a.e, we know from (A-2) of Assumptions (5.2.1) that $\mathbf{B}(\cdot)$ is positive definite a.e. Define the functional

$$\mathcal{M}(\mathbf{A}) = \int_0^1 \mathbf{B}(t) : \mathbf{A}^{-1}(t)dt \quad (5.98)$$

over the set $\mathbf{L}_a^1(0, 1)$. Then (5.97) becomes

$$\mathcal{M}(\mathbf{A}) \leq \liminf_{k \rightarrow \infty} \mathcal{M}(\mathbf{A}_k). \quad (5.99)$$

Note that $\mathbf{L}_a^1(0, 1)$ is a convex subset of the space $\mathbf{L}^1(0, 1)$. We first claim that the functional

\mathcal{M} is convex on $\mathbf{L}_a^1(0, 1)$. In fact, for any $\mathbf{A}_1, \mathbf{A}_2 \in \mathbf{L}_a^1(0, 1)$, $\alpha \in (0, 1)$,

$$\begin{aligned} \mathcal{M}(\alpha \mathbf{A}_1 + (1 - \alpha) \mathbf{A}_2) &= \int_0^1 \text{Tr} \left(\mathbf{B}(t) (\alpha \mathbf{A}_1(t) + (1 - \alpha) \mathbf{A}_2(t))^{-1} \right) dt \\ &= \int_0^1 \text{Tr} \left(\alpha \mathbf{A}_1(t) \mathbf{B}^{-1}(t) + (1 - \alpha) \mathbf{A}_2(t) \mathbf{B}^{-1}(t) \right)^{-1} dt \\ &\leq \alpha \int_0^1 \text{Tr}(\mathbf{A}_1(t) \mathbf{B}^{-1}(t))^{-1} dt + (1 - \alpha) \int_0^1 \text{Tr}(\mathbf{A}_2(t) \mathbf{B}^{-1}(t))^{-1} dt \\ &= \alpha \mathcal{M}(\mathbf{A}_1) + (1 - \alpha) \mathcal{M}(\mathbf{A}_2), \end{aligned}$$

where we used the trace inequality $\text{Tr}((\mathbf{C} + \mathbf{D})^{-1}) \leq \text{Tr}(\mathbf{C}^{-1}) + \text{Tr}(\mathbf{D}^{-1})$ for positive definite matrices \mathbf{C}, \mathbf{D} . Now we prove (5.99) by employing the convexity of \mathcal{M} . First by passing a subsequence (without relabelling), we may assume that $\mathcal{M}(\mathbf{A}_k)$ converges to θ . According to Mazur's Lemma 5.7.16, there exists a convex combination of $\{\mathbf{A}_k\}$, defined by

$$\bar{\mathbf{A}}_j = \sum_{k=j}^{N(j)} \alpha_{j,k} \mathbf{A}_k, \quad \alpha_{j,k} \in [0, 1], \quad \sum_{k=j}^{N(j)} \alpha_{j,k} = 1,$$

such that $\bar{\mathbf{A}}_j \rightarrow A$ strongly in $\mathbf{L}^1(0, 1)$. Note that we applied Mazur's Lemma 5.7.16 to the sequence $\{\mathbf{A}_k\}_{k \geq j}$ at step j . Since \mathcal{M} is convex, we obtain

$$\mathcal{M}(\bar{\mathbf{A}}_j) = \mathcal{M} \left(\sum_{k=j}^{N(j)} \alpha_{j,k} \mathbf{A}_k \right) \leq \sum_{k=j}^{N(j)} \alpha_{j,k} \mathcal{M}(\mathbf{A}_k).$$

Letting $j \rightarrow \infty$, since $k \geq j$ in the sum and $\mathcal{M}(\mathbf{A}_k) \rightarrow \theta$, we have

$$\liminf_{j \rightarrow \infty} \mathcal{M}(\bar{\mathbf{A}}_j) \leq \theta = \liminf_{k \rightarrow \infty} \mathcal{M}(\mathbf{A}_k). \quad (5.100)$$

In addition, it holds that

$$\mathcal{M}(\bar{\mathbf{A}}_j) \rightarrow \mathcal{M}(\mathbf{A}). \quad (5.101)$$

Indeed, since $m \in \mathbf{BV}(0, 1; \mathcal{E})$ and $\bar{\mathbf{A}}_j \rightarrow \mathbf{A}$ in $\mathbf{L}^1(0, 1)$,

$$\begin{aligned}
|\mathcal{M}(\mathbf{A} - \bar{\mathbf{A}}_j)| &= \left| \int_0^1 \text{Tr} \left(D^2 V(m(t)) (\mathbf{A}^{-1}(t) - \bar{\mathbf{A}}_j^{-1}(t)) \right) dt \right| \\
&\leq \int_0^1 \left| \text{Tr} \left(D^2 V(m(t)) \mathbf{A}^{-1}(t) (\bar{\mathbf{A}}_j(t) - \mathbf{A}(t)) \bar{\mathbf{A}}_j^{-1}(t) \right) \right| dt \\
&\lesssim \int_0^1 \left| D^2 V(m(t)) \mathbf{A}^{-1}(t) (\bar{\mathbf{A}}_j(t) - \mathbf{A}(t)) \bar{\mathbf{A}}_j^{-1}(t) \right|_F dt \\
&\lesssim \int_0^1 |D^2 V(m(t))|_F |\mathbf{A}^{-1}(t)|_F |\bar{\mathbf{A}}_j(t) - \mathbf{A}(t)|_F |\bar{\mathbf{A}}_j^{-1}(t)|_F dt \\
&\lesssim \|\bar{\mathbf{A}}_j(t) - \mathbf{A}(t)\|_{\mathbf{L}^1(0,1)} \rightarrow 0.
\end{aligned}$$

Therefore (5.99) follows from (5.100) and (5.101) and thereby proves (5.96).

Taking account of the fact that E_ε Γ -converges to E , we obtain from Proposition 5.4.3, (5.94) and (5.96) that

$$\begin{aligned}
\liminf_{\varepsilon \rightarrow 0} F_\varepsilon(m_\varepsilon, \mathbf{A}_\varepsilon) &= \lim_{k \rightarrow \infty} F_{\varepsilon_k}(m_{\varepsilon_k}, \mathbf{A}_{\varepsilon_k}) \\
&\geq E(m) + \frac{1}{4} \int_0^1 (D^2 V(m(t)) - \mathbf{A}(t))^2 : \mathbf{A}^{-1}(t) dt = F(m, \mathbf{A}).
\end{aligned}$$

Next we prove the limsup inequality, i.e. for a subsequence $\varepsilon_k \rightarrow 0$, we want to find a pair of recovering sequence (m_k, \mathbf{A}_k) converging to (m, \mathbf{A}) such that

$$\limsup_{k \rightarrow \infty} F_{\varepsilon_k}(m_k, \mathbf{A}_k) \leq F(m, \mathbf{A}).$$

It suffices to deal with the case where $F(m, \mathbf{A}) < \infty$ and hence $m(t) \in \mathcal{E}$. Otherwise the limsup inequality is automatically satisfied. First thanks to the Γ -convergence of E_ε to E , one automatically obtains a recovering sequence $m_k \in \mathbf{H}_\pm^1(0, 1)$ such that $m_k \rightarrow m$ in $\mathbf{L}^1(0, 1)$, $\limsup_k \|m_k\|_{\mathbf{L}^\infty(0,1)} < \infty$ and $\limsup_{k \rightarrow \infty} E_\varepsilon(m_k) \leq E(m)$. We construct a recovering sequence $\mathbf{A}_k \in \mathbf{H}_a^1(0, 1)$ explicitly by using convolution approximation. Specifically fixing any $\alpha < \gamma/3$, we define

$$\mathbf{A}_k := \tilde{\mathcal{K}}_{\varepsilon_k^\alpha} \mathbf{A} \tag{5.102}$$

where $\tilde{\mathcal{K}}_\varepsilon$ is the convolution operator defined in (5.126). It is proved in Lemma 5.7.14 that $\mathbf{A}_k \in \mathbf{H}_a^1(0, 1)$ and $\mathbf{A}_k \rightarrow \mathbf{A}$ in $\mathbf{L}^1(0, 1)$. Moreover, by replacing ε with ε^α in the bound proved in Lemma 5.7.14, we have

$$\varepsilon_k^\gamma \|\mathbf{A}_k\|_{\mathbf{H}^1(0,1)}^2 \lesssim \varepsilon_k^{\gamma-3\alpha} \rightarrow 0. \tag{5.103}$$

With the above choices for m_k and \mathbf{A}_k , we get from Proposition 5.4.3 that

$$\begin{aligned}
& \limsup_{k \rightarrow \infty} F_{\varepsilon_k}(m_k, \mathbf{A}_k) \\
&= \limsup_{k \rightarrow \infty} \left\{ E_{\varepsilon_k}(m_k, \mathbf{A}_k) \right. \\
&\quad + \frac{1}{4} \int_0^1 (D^2 V(m_k(t)) - \mathbf{A}_k(t))^2 : \mathbf{A}_k^{-1}(t) dt \\
&\quad \left. + \int_0^1 (D^3 V(m_k(t)) \cdot \nabla V(m_k(t))) : \mathbf{A}_k^{-1}(t) dt + \varepsilon_k^\gamma \|\mathbf{A}_k\|_{\mathbf{H}^1(0,1)}^2 \right\} \\
&\leq E(m) + \frac{1}{4} \int_0^1 (D^2 V(m_k(t)) - \mathbf{A}_k(t))^2 : \mathbf{A}_k^{-1}(t) dt \\
&= F(m, \mathbf{A}).
\end{aligned}$$

To pass to the inequality we have used the dominated convergence theorem and (5.94) for the third term on the left hand side as well as (5.103) for the fourth term on the left hand side. The proof is now complete. \square

Proof of Corollary 5.4.6. Let $(m_\varepsilon, \mathbf{A}_\varepsilon) \in \mathcal{H}$ be a minimiser of F_ε . We first argue that $\limsup_\varepsilon F_\varepsilon(m_\varepsilon, \mathbf{A}_\varepsilon) < \infty$. In fact, for any fixed $m \in \mathbf{BV}(0, 1; \mathcal{E})$ and $\mathbf{A} \in \mathbf{L}_a^1(0, 1)$, we know from the proof of the limsup inequality of Theorem 5.4.5 that there exists a recovering sequence $(\tilde{m}_\varepsilon, \tilde{\mathbf{A}}_\varepsilon)$ such that $\limsup_\varepsilon F_\varepsilon(\tilde{m}_\varepsilon, \tilde{\mathbf{A}}_\varepsilon) < \infty$. Since $(m_\varepsilon, \mathbf{A}_\varepsilon)$ minimises F_ε , we have

$$\limsup_{\varepsilon \rightarrow 0} F_\varepsilon(m_\varepsilon, \mathbf{A}_\varepsilon) \leq \limsup_{\varepsilon \rightarrow 0} F_\varepsilon(\tilde{m}_\varepsilon, \tilde{\mathbf{A}}_\varepsilon) < \infty.$$

Then by Proposition 5.4.4, there exists a subsequence ε_k and the corresponding $\{(m_k, \mathbf{A}_k)\} \subset \mathcal{H}$ such that $m_k \rightarrow m$ in $\mathbf{L}^1(0, 1)$ and $\mathbf{A}_k \rightharpoonup \mathbf{A}$ in $\mathbf{L}^1(0, 1)$ with some $m \in \mathbf{BV}(0, 1; \mathcal{E})$ and $\mathbf{A} \in \mathbf{L}_a^1(0, 1)$. We now show that (m, \mathbf{A}) minimises F . In fact, given any $\tilde{m} \in \mathbf{BV}(0, 1; \mathcal{E})$ and $\tilde{\mathbf{A}} \in \mathbf{L}_a^1(0, 1)$, thanks to the Γ -convergence of F_ε to F , one can find a recovering sequence $(\tilde{m}_k, \tilde{\mathbf{A}}_k) \in \mathcal{H}$ such that

$$\limsup_k F_{\varepsilon_k}(\tilde{m}_k, \tilde{\mathbf{A}}_k) \leq F(\tilde{m}, \tilde{\mathbf{A}}).$$

Since (m_k, \mathbf{A}_k) minimises F_{ε_k} , we have $F_{\varepsilon_k}(m_k, \mathbf{A}_k) \leq F_{\varepsilon_k}(\tilde{m}_k, \tilde{\mathbf{A}}_k)$. Then using the liminf inequality part of the Γ -convergence of F_ε to F , we obtain

$$F(m, \mathbf{A}) \leq \liminf_{k \rightarrow \infty} F_{\varepsilon_k}(m_k, \mathbf{A}_k) \leq \limsup_{k \rightarrow \infty} F_{\varepsilon_k}(\tilde{m}_k, \tilde{\mathbf{A}}_k) \leq F(\tilde{m}, \tilde{\mathbf{A}}).$$

Since $\tilde{m}, \tilde{\mathbf{A}}$ is arbitrary, (m, \mathbf{A}) is a minimiser of F . \square

5.7 Appendix

5.7.1 Estimates on The Constant Coefficient Green's Functions

Assume that function $|\lambda(t)| \geq a$ almost everywhere in $[0, 1]$ with some $a > 0$. For any $s \in (0, 1)$, let $\overline{G}_\varepsilon^\lambda$ be the solution to the equation

$$\begin{aligned} (-\partial_t^2 + \varepsilon^{-2}\lambda^2(s)) \overline{G}_\varepsilon^\lambda(t, s) &= \delta(t - s), \quad t \in (0, 1), \\ \overline{G}_\varepsilon^\lambda(0, s) &= \overline{G}_\varepsilon^\lambda(1, s) = 0, \end{aligned} \quad (5.104)$$

where δ is the Dirac function. The solution $\overline{G}_\varepsilon^\lambda$ is given explicitly as follows

$$\overline{G}_\varepsilon^\lambda(t, s) = \frac{\varepsilon}{|\lambda(s)| \sinh(|\lambda(s)|/\varepsilon)} \times \begin{cases} \sinh(|\lambda(s)|s/\varepsilon) \sinh(|\lambda(s)|(1-t)/\varepsilon) & s \leq t; \\ \sinh(|\lambda(s)|t/\varepsilon) \sinh(|\lambda(s)|(1-s)/\varepsilon) & s \geq t. \end{cases}$$

Notice that $\overline{G}_\varepsilon^\lambda(t, s)$ is not a standard Green's function as it is not symmetric with respect to permutation of its arguments. According to the definition of \sinh , a few elementary calculations yield the following estimates.

Lemma 5.7.1. *Let $|\lambda(t)| \geq a$ a.e. on $(0, 1)$ for a fixed $a > 0$. Then for sufficiently small $\varepsilon > 0$, the solution $\overline{G}_\varepsilon^\lambda$ to the equation (5.104) satisfies the following.*

(i) *There exists $C = C(a) > 0$ such that*

$$0 \leq \overline{G}_\varepsilon^\lambda(t, s) \leq C\varepsilon e^{-\frac{a}{\varepsilon}|s-t|} \quad (5.105)$$

for any $t, s \in [0, 1]$.

(ii) *There exists $C = C(a) > 0$ such that*

$$\overline{G}_\varepsilon^\lambda(t, t) = \frac{\varepsilon}{2} \left(\frac{1}{|\lambda(t)|} + R(t) \right), \quad t \in [0, 1]$$

with

$$|R(t)| \leq C \left(e^{-\frac{2at}{\varepsilon}} + e^{-\frac{2a(1-t)}{\varepsilon}} \right). \quad (5.106)$$

Considering the Green's tensor $\overline{\mathbf{G}}_\varepsilon(t, s)$ that solves the matrix equation

$$\begin{aligned} (-\partial_t^2 + \varepsilon^{-2}\mathbf{A}(s)) \overline{\mathbf{G}}_\varepsilon(\cdot, s) &= \delta(\cdot - s) \cdot \mathbf{I}_d, \\ \overline{\mathbf{G}}_\varepsilon(0, s) &= \overline{\mathbf{G}}_\varepsilon(1, s) = 0, \end{aligned} \quad (5.107)$$

with $\mathbf{A} \in \mathbf{H}^1(0, 1)$ and $|\mathbf{A}| \geq a$ a.e. on $(0, 1)$, we have the following similar estimates.

Lemma 5.7.2. *Let $\mathbf{A} \in \mathbf{H}^1(0, 1)$ and $|\mathbf{A}| \geq a$ a.e. on $(0, 1)$. For sufficiently small $\varepsilon > 0$, the solution $\overline{\mathbf{G}}_\varepsilon$ to the equation (5.107) satisfies the following.*

(i) *there exists $C = C(a) > 0$ such that*

$$|\overline{\mathbf{G}}_\varepsilon(t, s)| \leq C\varepsilon e^{-\frac{a}{\varepsilon}|s-t|} \quad (5.108)$$

for any $t, s \in [0, 1]$.

(ii) *there exists $C = C(a) > 0$ such that*

$$\overline{\mathbf{G}}_\varepsilon(t, t) = \frac{\varepsilon}{2} (|\mathbf{A}^{-1}(t)| + \mathbf{R}(t)) \quad (5.109)$$

with

$$|\mathbf{R}(t)| \leq C \left(e^{-\frac{2at}{\varepsilon}} + e^{-\frac{2a(1-t)}{\varepsilon}} \right). \quad (5.110)$$

Proof. Since $\mathbf{A}(s)$ is symmetric for any $s \in (0, 1)$ (by the definition of $\mathbf{H}^1(0, 1)$), there exists an orthogonal matrix $\mathbf{P}(s)$ such that $\mathbf{A}(s) = \mathbf{P}^{-1}(s)\mathbf{\Lambda}(s)\mathbf{P}(s)$ where $\mathbf{\Lambda}(s) = \text{diag}(\lambda_1(s), \dots, \lambda_d(s))$. Moreover, by assumption we have $|\lambda_i(s)| \geq a$ a.e. on $(0, 1)$ for any $i = 1, \dots, d$. Therefore, the problem (5.107) can be diagonalised so that one obtains

$$\overline{\mathbf{G}}_\varepsilon(t, s) = \mathbf{P}^{-1}(s) \cdot \text{diag}(\overline{G}_\varepsilon^{\lambda_1}(t, s), \dots, \overline{G}_\varepsilon^{\lambda_d}(t, s)) \cdot \mathbf{P}(s), \quad (5.111)$$

where $\overline{G}_\varepsilon^{\lambda_i}(\cdot, s)$ solves (5.104) with λ replaced by λ_i . Then (5.108) follows directly from (5.111) and equation (5.105), and (5.109) can be deduced from (5.111) and (5.106). \square

5.7.2 Fundamental Matrix of Linear Systems

Given $f : \mathbf{R} \rightarrow \mathbf{R}^d$ and $\mathbf{A} : \mathbf{R} \rightarrow \mathbf{R}^{d \times d}$, consider the following linear differential equation

$$dx_\varepsilon(t) = -\varepsilon^{-1}\mathbf{A}(t)x_\varepsilon(t)dt + f(t)dt, \quad x_\varepsilon(t_0) = 0. \quad (5.112)$$

The solution to (5.112) can be found via the variation of constants method provided its fundamental matrix is determined.

Definition 5.7.3 (Fundamental matrix). *The fundamental matrix $\mathbf{M}_\varepsilon(t, t_0)$ is the solution*

matrix that solves the problem

$$\frac{d}{dt}\mathbf{M}_\varepsilon(t, t_0) = -\varepsilon^{-1}\mathbf{A}(t)\mathbf{M}_\varepsilon(t, t_0), \quad \mathbf{M}_\varepsilon(t_0, t_0) = \mathbf{I}_d. \quad (5.113)$$

Suppose that \mathbf{A} and f are both continuous, then the solution to the ODE (5.112) can be written in the form

$$x_\varepsilon(t) = \int_{t_0}^t \mathbf{M}_\varepsilon(t, s)f(s)ds.$$

We comment that the above formula is still valid when $f(s)ds$ is replaced by $dW(s)$, in which case the integral is understood as Itô's stochastic integration. In the case that $d = 1$ or if \mathbf{A} does not depend on t , we have $\mathbf{M}_\varepsilon(t, s) = \exp\left(-\varepsilon^{-1} \int_s^t \mathbf{A}(r)dr\right)$. In general, there is no closed form expression for the fundamental matrix \mathbf{M}_ε and hence the solution to (5.112) has no explicit formula. Nevertheless, \mathbf{M}_ε has some nice properties which are useful to study the asymptotic behaviour of the solution to (5.112) when $\varepsilon \rightarrow 0$.

Lemma 5.7.4. *Let \mathbf{M}_ε be the fundamental matrix defined by (5.113). Then we have*

- (i) *For all $t, t_0, t_1 \in \mathbf{R}$, $\mathbf{M}_\varepsilon(t, t_0) = \mathbf{M}_\varepsilon(t, t_1)\mathbf{M}_\varepsilon(t_1, t_0)$.*
- (ii) *For all $t, t_0 \in \mathbf{R}$, $\mathbf{M}_\varepsilon(t, t_0)$ is non-singular and $\mathbf{M}_\varepsilon^{-1}(t, t_0) = \mathbf{M}_\varepsilon(t_0, t)$.*
- (iii) *For all $t, t_0 \in \mathbf{R}$,*

$$\det(\mathbf{M}_\varepsilon(t, t_0)) = \exp\left(-\varepsilon^{-1} \int_{t_0}^t \text{Tr}(\mathbf{A}(s))ds\right). \quad (5.114)$$

Proof. The proof can be found in [28, Chapter 6]. □

We finish this appendix with two useful inequalities about the determinants of symmetric positive definite matrices.

Lemma 5.7.5. *If \mathbf{A}, \mathbf{B} are real symmetric positive definite matrices of size d , then*

$$(\det(\mathbf{A} + \mathbf{B}))^{\frac{1}{d}} \geq (\det(\mathbf{A}))^{\frac{1}{d}} + (\det(\mathbf{B}))^{\frac{1}{d}}. \quad (5.115)$$

A proof of this lemma can be found in [163, Page 115]. It shows that the function $\mathbf{A} \mapsto \det(\mathbf{A})^{\frac{1}{d}}$ is concave. As a consequence, we have the following corollary.

Corollary 5.7.6. *Suppose that $\mathbf{A} \in C([0, 1]; \mathbf{R}^{d \times d})$ is a matrix-valued function and that $\mathbf{A}(t)$ is symmetric positive definite for any $t \in [0, 1]$. Then we have*

$$\left[\det \left(\int_0^1 \mathbf{A}(t)dt \right) \right]^{\frac{1}{d}} \geq \int_0^1 \det(\mathbf{A}(t))^{\frac{1}{d}} dt. \quad (5.116)$$

Proof. Define $t_i = i/N$ with $i = 0, 1, \dots, N$. Since \mathbf{A} is continuous on $[0, 1]$, it holds that

$$\begin{aligned} \left[\det \left(\int_0^1 \mathbf{A}(t) dt \right) \right]^{\frac{1}{d}} &= \lim_{N \rightarrow \infty} \left[\det \left(\frac{1}{N} \sum_{i=1}^N \mathbf{A}(t_i) \right) \right]^{\frac{1}{d}} \\ &= \lim_{N \rightarrow \infty} \frac{1}{N} \left[\det \left(\sum_{i=1}^N \mathbf{A}(t_i) \right) \right]^{\frac{1}{d}} \\ &\geq \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N \det(\mathbf{A}(t_i))^{\frac{1}{d}} = \int_0^1 \det(\mathbf{A}(t))^{\frac{1}{d}} dt. \end{aligned}$$

We have used (5.115) in the inequality. \square

5.7.3 Useful Inequalities and Lemmas

Lemma 5.7.7 (Interpolation inequality). *Let $u \in H_0^1(0, 1)$. Then*

$$\|u\|_{H^s} \lesssim \|u\|_{H^1}^s \|u\|_{L^2}^{1-s} \quad (5.117)$$

for any $s \in [0, 1]$.

Proof. See [110, Corollary 6.11] for the proof. \square

Lemma 5.7.8. *Let $u \in H_0^1(0, 1)$. Then $\|u\|_{L^\infty}^2 \leq 2\|u\|_{L^2}|u|_{H^1}$.*

Proof. It suffices to prove the inequality when $u \in C_0^\infty(0, 1)$. For any $t \in (0, 1)$, it follows from the fundamental theorem of calculus and Cauchy-Schwarz inequality that

$$u^2(t) = 2 \int_0^t u(s)u'(s)ds \leq 2\|u\|_{L^2}|u|_{H^1}. \quad (5.118)$$

The lemma then follows by taking the supremum over t . \square

Lemma 5.7.9. *Let $\alpha, \beta \in (0, 1)$ be such that $\beta > \max(\alpha, \alpha/2 + 1/4)$. Then any matrix-valued function $B \in \mathbf{H}^{-\alpha}(0, 1)$ can be viewed as a bounded multiplication operator from \mathbf{H}_0^β to $\mathbf{H}^{-\beta}$. Furthermore we have*

$$\|B\|_{\mathcal{L}(\mathbf{H}_0^\beta, \mathbf{H}^{-\beta})} \lesssim \|B\|_{\mathbf{H}^{-\alpha}(0, 1)}. \quad (5.119)$$

Proof. It suffices to consider the proof in the scalar case. Let $B \in H^{-\alpha}$ and $\varphi \in H_0^\beta$. Assume that $\beta > \alpha$, then one can define the multiplication $B\varphi$ as a distribution in the sense that for any $\psi \in C_0^\infty(0, 1)$,

$$\langle B\varphi, \psi \rangle = \langle B, \varphi\psi \rangle.$$

Moreover, if $\beta - \alpha/2 > 1/4$, we have

$$|\langle B\varphi, \psi \rangle| = |\langle B, \varphi\psi \rangle| \leq \|B\|_{H^{-\alpha}} \|\varphi\psi\|_{H^\alpha} \lesssim \|B\|_{H^{-\alpha}} \|\varphi\|_{H^\beta} \|\psi\|_{H^\beta}$$

where the last estimate follows from the following Lemma. Therefore the desired estimate (5.119) holds. \square

Lemma 5.7.10. *Let α, β and γ be positive exponents such that $\min(\alpha, \beta) > \gamma$ and $\alpha + \beta > \gamma + 1/2$. Then, if $\varphi \in H^\alpha$ and $\psi \in H^\beta$, the product $\varphi\psi$ belongs to H^γ and $\|\varphi\psi\|_{H^\gamma} \lesssim \|\varphi\|_{H^\alpha} \|\psi\|_{H^\beta}$.*

Proof. The proof can be found in [110, Theorem 6.18]. \square

Lemma 5.7.11. *Let $A \in H^1(0, 1)$ and let $f \in L^2(0, 1)$. Set $B = A^2 - A'$. Then there exists a unique solution $u \in H_0^1(0, 1)$ solving the problem*

$$\begin{aligned} (-\partial_t^2 + B)u &= f \text{ on } (0, 1), \\ u(0) &= u(1) = 0. \end{aligned} \tag{5.120}$$

Moreover, it holds that

$$\|u\|_{H^2(0,1)} \leq C\|f\|_{L^2(0,1)}, \tag{5.121}$$

and $(-\partial_t^2 + B)^{-1}$ is a trace-class operator on $L^2(0, 1)$.

Proof. Let $G_0(s, t)$ be the Dirichlet Green's function of $-\partial_t^2$ on $(0, 1)$. In fact, $G_0(s, t) = s(1-t) \wedge t(1-s)$ for all $s, t \in [0, 1]$. From Green's first identity, it is easy to observe that a solution $u \in H_0^1(0, 1)$ solving (5.120) is a solution $u \in L^2(0, 1)$ that solves the Lippmann-Schwinger integral equation

$$u(t) + \int_0^1 G_0(t, s)B(s)u(s)ds = \int_0^1 G_0(t, s)f(s)ds \tag{5.122}$$

and vice versa. Now we apply the Fredholm alternative theorem to prove the existence and uniqueness of solution to (5.122). First the operator

$$(\mathcal{T}u)(t) := (-\partial_t^2)^{-1}(Bu)(t) = \int_0^1 G_0(t, s)B(s)u(s)ds$$

is compact from $L^2(0, 1)$ to itself. There are several ways to prove this, but the simplest argument is perhaps the observation that \mathcal{T} is bounded from $L^2(0, 1)$ to $W^{1,\infty}(0, 1)$. Indeed, since $G_0(t, \cdot) \in W^{1,\infty}(0, 1)$ for any $t \in [0, 1]$, we can apply Cauchy-Schwarz inequality

twice to get

$$\begin{aligned}\|\mathcal{T}u\|_{W^{1,\infty}(0,1)} &\leq \sup_{t \in [0,1]} \|G_0(t, \cdot)\|_{W^{1,\infty}(0,1)} \|Bu\|_{L^1(0,1)} \\ &\leq \sup_{t \in [0,1]} \|G_0(t, \cdot)\|_{W^{1,\infty}(0,1)} \|B\|_{L^2(0,1)} \|u\|_{L^2(0,1)}.\end{aligned}\tag{5.123}$$

Then the compactness of \mathcal{T} follows from the compact embedding $W^{1,\infty}(0,1) \hookrightarrow L^2(0,1)$. We are left to show the uniqueness of (5.122) or equivalently (5.120). To see this, setting $f = 0$, we multiply the equation (5.120) by u , integrate, use Green's first identity and get

$$\begin{aligned}0 &= \int_0^1 u'(t)^2 dt + \int_0^1 (A^2(t) - A'(t)) u^2(t) dt \\ &= \int_0^1 u'(t)^2 dt + \int_0^1 A^2(t) u^2(t) dt + 2 \int_0^1 A(t) u(t) u'(t) dt \\ &= \int_0^1 (u'(t) + A(t)u(t))^2 dt.\end{aligned}$$

Therefore we should have $u'(t) = -A(t)u(t)$. The only solution to this equation with the Dirichlet boundary conditions is zero. Hence by the Fredholm alternative theorem, the integral equation (5.122) has a unique solution in $L^2(0,1)$. Then the estimate (5.121) follows from (5.123), (5.122) and estimate that $\|\mathcal{R}f\|_{H^2(0,1)} \leq C\|f\|_{L^2(0,1)}$ where

$$(\mathcal{R}f)(t) = \int_0^1 G_0(t, s) f(s) ds.$$

Finally observe that

$$(-\partial_t^2 + B)^{-1} = (I + (-\partial_t^2)^{-1}B)^{-1}(-\partial_t^2)^{-1} = (I + \mathcal{T})^{-1}(-\partial_t^2)^{-1}.$$

Then it follows from the fact that $(-\partial_t^2)^{-1}$ is a trace-class operator on $L^2(0,1)$ and the boundedness of $(I + \mathcal{T})^{-1}$ that $(-\partial_t^2 + B)^{-1}$ is trace-class. \square

Remark 5.7.12. Lemma 5.7.11 can be easily extended to the matrix-valued case. More precisely, assume that $\mathbf{A} \in \mathbf{H}^1(0,1)$ and $\mathbf{A}(t)$ is a symmetric matrix for any $t \in [0,1]$. Let $\mathbf{B} = \mathbf{A}^2 - \mathbf{A}'$. Then the inverse of the matrix-valued Schrödinger operator $(-\partial_t^2 + \mathbf{B})^{-1}$ is bounded from $\mathbf{L}^2(0,1)$ to $\mathbf{H}^2(0,1)$ and is a trace-class operator on $\mathbf{L}^2(0,1)$. \square

The next lemma discusses some properties of approximation by convolution.

Lemma 5.7.13. Let $K \in C_0^\infty(\mathbf{R})$ such that $K \geq 0$ and $\int_{\mathbf{R}} K = 1$. Denote by $K_\varepsilon(\cdot) = \varepsilon^{-1}K(x/\varepsilon)$. Suppose that $f \in L^1(\mathbf{R})$ and define $\mathcal{K}_\varepsilon f = K_\varepsilon * f$. Then $\mathcal{K}_\varepsilon f \in L^1(\mathbf{R})$ and

$C^\infty(\mathbf{R})$. Moreover, we have

$$\mathcal{K}_\varepsilon f \rightarrow f \quad \text{in } L^1(\mathbf{R}) \quad (5.124)$$

and

$$\|\mathcal{K}_\varepsilon f\|_{H^1(\mathbf{R})} \leq C\varepsilon^{-\frac{3}{2}}\|f\|_{L^1(\mathbf{R})}. \quad (5.125)$$

Proof. The property (5.124), often termed as the approximation of identity in $\mathcal{L}^1(\mathbf{R})$, has been proved in many books, e.g. [38]. We now show that $\mathcal{K}_\varepsilon f \in H^1(\mathbf{R})$ and that (5.125) is valid. This can be seen from the observation that

$$\begin{aligned} \|\mathcal{K}_\varepsilon f\|_{H^1(\mathbf{R})}^2 &= \|\mathcal{K}_\varepsilon f\|_{L^2(\mathbf{R})}^2 + \|\mathcal{K}'_\varepsilon f\|_{L^2(\mathbf{R})}^2 \\ &= \|\varepsilon^{-1}K(\cdot/\varepsilon) * f\|_{L^2(\mathbf{R})}^2 + \varepsilon^{-2}\|\varepsilon^{-1}K'(\cdot/\varepsilon) * f\|_{L^2(\mathbf{R})}^2 \\ &\leq \varepsilon^{-1}\|K\|_{L^2(\mathbf{R})}^2\|f\|_{L^1(\mathbf{R})}^2 + \varepsilon^{-3}\|K'\|_{L^2(\mathbf{R})}^2\|f\|_{L^1(\mathbf{R})}^2 \leq C\varepsilon^{-3}\|f\|_{L^1(\mathbf{R})}^2. \end{aligned}$$

Note that we have used Young's inequalities in the penultimate inequality. \square

We continue to adapt Lemma (5.7.13) to matrix functions defined on a bounded domain. For this purpose, we define two useful operators. Given a function $f \in L^1(0, 1)$, we define its extension

$$\mathcal{E}f(x) := \begin{cases} f(x) & \text{if } x \in (0, 1), \\ 0 & \text{otherwise.} \end{cases}$$

Conversely, for a function $g \in L^1(\mathbf{R})$, we define the restriction $\mathcal{R}f := f|_{(0,1)}$. Likewise, we can define the convolution, extension or restriction of a matrix function through entry-wise operations. The following lemma concerns the convolution approximation of matrix-valued functions.

Lemma 5.7.14. *Let $\mathbf{A} \in \mathbf{L}_a^1(0, 1)$. Define*

$$\tilde{\mathcal{K}}_\varepsilon \mathbf{A} := \mathcal{R}(\mathcal{K}_\varepsilon(\mathcal{E}(\mathbf{A} - a \cdot \mathbf{I}_d)) + a \cdot \mathbf{I}_d). \quad (5.126)$$

Then $\tilde{\mathcal{K}}_\varepsilon \mathbf{A} \in \mathbf{H}_a^1(0, 1)$. Moreover, $\tilde{\mathcal{K}}_\varepsilon \mathbf{A} \rightarrow \mathbf{A}$ in $\mathbf{L}^1(0, 1)$ and $\|\tilde{\mathcal{K}}_\varepsilon \mathbf{A}\|_{\mathbf{H}^1(0,1)} \leq C\varepsilon^{-\frac{3}{2}}$ with the constant C depending on A and a .

Proof. First it follows from Lemma (5.7.13) that $\tilde{\mathcal{K}}_\varepsilon \mathbf{A} \in \mathbf{H}^1(0, 1)$. To show $\tilde{\mathcal{K}}_\varepsilon \mathbf{A} \in \mathbf{H}_a^1(0, 1)$, it suffices to show $\mathcal{K}_\varepsilon(\mathcal{E}(\mathbf{A} - a \cdot \mathbf{I}_d))$ is positive semi-definite. Indeed, for any

fixed $x \in \mathbf{R}^d$,

$$\begin{aligned} x^T \mathcal{K}_\varepsilon (\mathcal{E}(\mathbf{A} - a \cdot \mathbf{I}_d)) x &= \mathcal{K}_\varepsilon (\mathcal{E}(x^T (\mathbf{A} - a \cdot \mathbf{I}_d) x)) \\ &= K_\varepsilon(\cdot) * \mathcal{E}(x^T (\mathbf{A}(\cdot) - a \cdot \mathbf{I}_d) x) \geq 0, \end{aligned}$$

where we have used the assumption that $\mathbf{A}(\cdot) - a \cdot \mathbf{I}_d$ is positive semi-definite a.e. on $(0, 1)$. Next from Lemma (5.7.13) and the fact that $\mathcal{E}(\mathbf{A} - a \cdot \mathbf{I}_d) \in \mathbf{L}^1(\mathbf{R})$, we have

$$\begin{aligned} \|\tilde{\mathcal{K}}_\varepsilon \mathbf{A} - \mathbf{A}\|_{\mathbf{L}^1(0,1)} &= \|\mathcal{R}(\mathcal{K}_\varepsilon (\mathcal{E}(\mathbf{A} - a \cdot \mathbf{I}_d)) - \mathcal{E}(\mathbf{A} - a \cdot \mathbf{I}_d))\|_{\mathbf{L}^1(0,1)} \\ &\leq \|\mathcal{K}_\varepsilon (\mathcal{E}(\mathbf{A} - a \cdot \mathbf{I}_d)) - \mathcal{E}(\mathbf{A} - a \cdot \mathbf{I}_d)\|_{\mathbf{L}^1(\mathbf{R})} \rightarrow 0. \end{aligned}$$

By similar arguments one can show that $\|\tilde{\mathcal{K}}_\varepsilon \mathbf{A}\|_{\mathbf{H}^1(0,1)} \leq C\varepsilon^{-\frac{3}{2}}$. \square

The next lemma characterises explicitly for the minimiser of the second component (as a functional of \mathbf{A}) of the functional F defined in (5.51). Recall the notation $|\mathbf{A}|$ of a matrix \mathbf{A} defined in Section 5.2.2.

Lemma 5.7.15. *Let \mathbf{B} be a fixed symmetric matrix. Let \mathbf{A} be a minimiser of the functional*

$$\mathcal{G}(\mathbf{A}) := (\mathbf{B} - \mathbf{A})^2 : \mathbf{A}^{-1}$$

over all positive matrices. Then it holds that $\mathbf{A} = |\mathbf{B}|$. With this choice of \mathbf{A} , $\mathcal{G}(\mathbf{A}) = 2(\text{Tr}(|\mathbf{B}|) - \text{Tr}(\mathbf{B}))$.

Proof. The lemma follows from the fact that the functional \mathcal{G} can be rewritten as

$$\begin{aligned} \mathcal{G}(\mathbf{A}) &= \text{Tr}(\mathbf{B}^2 \mathbf{A}^{-1}) + \text{Tr}(\mathbf{A}) - 2\text{Tr}(\mathbf{B}) \\ &= \text{Tr}(\mathbf{B}^2 \mathbf{A}^{-1}) + \text{Tr}(\mathbf{A}) - 2\text{Tr}(|\mathbf{B}|) + 2\text{Tr}(|\mathbf{B}|) - 2\text{Tr}(\mathbf{B}) \\ &= \text{Tr}((|\mathbf{B}| - \mathbf{A})^2 \mathbf{A}^{-1}) + 2\text{Tr}(|\mathbf{B}|) - 2\text{Tr}(\mathbf{B}) \\ &= (|\mathbf{B}| - \mathbf{A})^2 : \mathbf{A}^{-1} + 2\text{Tr}(|\mathbf{B}|) - 2\text{Tr}(\mathbf{B}). \end{aligned}$$

\square

Finally the following Mazur's Lemma is useful to obtain a strong convergent subsequence from a weakly convergent sequence. The proof can be found in [30, Corollary 3.8].

Lemma 5.7.16. (Mazur's lemma) *Let X be a Banach space and let $\{u_n\}_{n \in \mathbb{N}}$ be a sequence in X that converges weakly to $u \in X$. Then there exists a sequence $\{\bar{u}_j\}_{j \in \mathbb{N}}$ defined by the*

convex combination of $\{u_n\}_{n \in \mathbb{N}}$, namely

$$\bar{u}_j = \sum_{n=1}^{N(j)} \alpha_{j,n} u_n, \quad \alpha_{j,n} \in [0, 1], \quad \sum_{n=1}^{N(j)} \alpha_{j,n} = 1, \quad (5.127)$$

such that \bar{u}_j converges to u strongly in X .

5.7.4 Proof of Proposition 5.4.2

We first show the liminf inequality. Suppose that $\{m_\varepsilon\} \subset \mathbf{H}_\pm^1(0, 1)$ and that $m_\varepsilon \rightarrow m$ in $\mathbf{L}^1(0, 1)$, we want to prove that $E(m) \leq \liminf_{\varepsilon \rightarrow 0} E_\varepsilon(m_\varepsilon)$. We may assume that $\liminf_{\varepsilon \rightarrow 0} E_\varepsilon(m_\varepsilon) < \infty$ since otherwise there is nothing to prove. Let $\{\varepsilon_n\}$ and $\{m_n\} \subset \mathbf{H}_\pm^1(0, 1)$ be subsequences such that $\varepsilon_n \rightarrow 0$ and that

$$\lim_{n \rightarrow \infty} E_{\varepsilon_n}(m_n) = \liminf_{\varepsilon \rightarrow 0} E_\varepsilon(m_\varepsilon) < \infty.$$

By Lemma 5.4.1, $m \in \mathbf{BV}(0, 1; \mathcal{E})$ and one can extract a further subsequence (without relabelling) such that $m_n(t) \rightarrow m(t)$ a.e. $t \in (0, 1)$. It is sufficient to deal with the case where m only has a single jump at $\tau \in (0, 1)$, i.e.

$$m(t) = \begin{cases} m(\tau^-), & \text{if } t \in (0, \tau), \\ m(\tau^+), & \text{if } t \in [\tau, 1). \end{cases} \quad (5.128)$$

Let $0 < t_1 < \tau < t_2 < 1$ and $m_n(t_1) \rightarrow m(t_1) = m(\tau^-)$, $m_n(t_2) \rightarrow m(t_2) = m(\tau^+)$. Define $\tilde{m}_n = m_n(\varepsilon_n^{-1}(t - (t_1 + t_2)/2))$. Then it follows from the equality (5.48) that

$$\begin{aligned} & \lim_{n \rightarrow \infty} \frac{1}{4} \int_{t_1}^{t_2} \varepsilon_n |m'_n(t)|^2 + \frac{1}{\varepsilon_n} |\nabla V(m_n(t))|^2 dt \\ &= \lim_{n \rightarrow \infty} \frac{1}{4} \int_{\frac{t_1 - t_2}{2\varepsilon_n}}^{\frac{t_2 - t_1}{2\varepsilon_n}} |\tilde{m}'_n(t)|^2 + |\nabla V(\tilde{m}_n(t))|^2 dt \\ &\geq \inf_{T, m} \left\{ \frac{1}{4} \int_{-T}^T |m'(t)|^2 + |\nabla V(m(t))|^2 dt : T > 0, m \in \mathbf{H}^1(-T, T) \text{ and} \right. \\ &\quad \left. m(-T) = x_-, m(T) = x_+ \right\} = \Phi(m(\tau^-), m(\tau^+)). \end{aligned}$$

Similarly, taking into account that m_n satisfies the end point conditions, one can obtain

$$\lim_{n \rightarrow \infty} \frac{1}{4} \int_0^{t_1} \varepsilon_n |m'_n(t)|^2 + \frac{1}{\varepsilon_n} |\nabla V(m_n(t))|^2 dt \geq \Phi(x_-, m(0^+))$$

and

$$\lim_{n \rightarrow \infty} \frac{1}{4} \int_{t_2}^1 \varepsilon_n |m'_n(t)|^2 + \frac{1}{\varepsilon_n} |\nabla V(m_n(t))|^2 dt \geq \Phi(m(1^-), x_+).$$

Therefore the liminf inequality $E(m) \leq \liminf_{\varepsilon \rightarrow 0} E_\varepsilon(m_\varepsilon)$ follows.

Now we prove the limsup inequality, and again it suffices to consider m defined by (5.128). According to the equation (5.48), for any small $\eta > 0$, there exists $T > 0$ and $m_i \in \mathbf{H}^1(-T, T)$, $i = 1, 2, 3$ such that

$$\begin{aligned} m_1(-T) &= x_-, m_1(T) = m(0^+) \text{ and } \mathcal{J}_T(m_1) \leq \Phi(x_-, m(0^+)) + \eta/3, \\ m_2(-T) &= m(\tau^-), m_2(T) = m(\tau^+) \text{ and } \mathcal{J}_T(m_2) \leq \Phi(m(\tau^-), m(\tau^+)) + \eta/3, \\ m_3(-T) &= m(1^-), m_3(T) = x_+ \text{ and } \mathcal{J}_T(m_3) \leq \Phi(m(1^-), x_+) + \eta/3. \end{aligned}$$

Then for $\varepsilon > 0$ small enough, we define the recovery sequence

$$m_\varepsilon(t) = \begin{cases} m_1(-T + \varepsilon^{-1}t) & \text{if } t \in (0, 2\varepsilon T), \\ m(0^+) & \text{if } t \in (2\varepsilon T, \tau - \varepsilon T), \\ m_2(\varepsilon^{-1}(t - \tau)) & \text{if } t \in (\tau - \varepsilon T, \tau + \varepsilon T), \\ m(1^-) & \text{if } t \in (\tau + \varepsilon T, 1 - 2\varepsilon T), \\ m_3(\varepsilon^{-1}(t - 1) + T) & \text{if } t \in (1 - 2\varepsilon T, 1). \end{cases}$$

It is clear that $m_\varepsilon \in \mathbf{H}_\pm^1(0, 1)$ and $m_\varepsilon \rightarrow m$ in $\mathbf{L}^1(0, 1)$ as $\varepsilon \rightarrow 0$. Furthermore, we have

$$\begin{aligned} & \limsup_{\varepsilon \rightarrow 0} E_\varepsilon(m_\varepsilon) \\ &= \limsup_{\varepsilon \rightarrow 0} \left\{ \frac{1}{4} \int_0^1 \varepsilon |m'_\varepsilon(t)|^2 + \frac{1}{\varepsilon} |\nabla V(m_\varepsilon(t))|^2 dt \right\} \\ &= \limsup_{\varepsilon \rightarrow 0} \left\{ \frac{1}{4} \int_0^{2\varepsilon T} \varepsilon |m'_\varepsilon(t)|^2 + \frac{1}{\varepsilon} |\nabla V(m_\varepsilon(t))|^2 dt \right. \\ & \quad \left. + \frac{1}{4} \int_{\tau - \varepsilon T}^{\tau + \varepsilon T} \varepsilon |m'_\varepsilon(t)|^2 + \frac{1}{\varepsilon} |\nabla V(m_\varepsilon(t))|^2 dt + \frac{1}{4} \int_{1 - 2\varepsilon T}^1 \varepsilon |m'_\varepsilon(t)|^2 + \frac{1}{\varepsilon} |\nabla V(m_\varepsilon(t))|^2 dt \right\} \\ &\leq \Phi(x_-, m(0^+)) + \Phi(m(\tau^-), m(\tau^+)) + \Phi(m(1^-), x_+) + \eta. \end{aligned}$$

Since η is arbitrary, the limsup inequality follows.

Chapter 6

A Bayesian Level Set Method for Geometric Inverse Problems

6.1 Introduction

Geometric inverse problems, in which the interfaces between different domains are the primary unknown quantities, are ubiquitous in applications including medical imaging problems such as EIT [23] and subsurface flow [8]; they also have an intrinsically interesting mathematical structure [129]. In many such applications the data is sparse, so that the problem is severely under-determined, and noisy. For both these reasons the Bayesian approach to the inverse problem is attractive as the probabilistic formulation allows for regularisation of the under-determined, and often ill-posed, inversion via the introduction of priors, and simultaneously deals with the presence of noise in the observations [136, 215]. The level set method has been a highly successful methodology for the solution of classical, non-statistical, inverse problems for interfaces since the seminal paper of Santosa [204]; see for example [5, 10, 35–37, 55, 70, 71, 128, 150, 151, 218, 223, 228] and for related Bayesian level set approaches see [154, 155, 186, 231]. For interface problems, the phase field approach [37, 64] is sometimes used as an alternative to the level set method; in this approach the recovered interfaces between different phases are smeared out. Also, recently the Bayesian framework of [215] is adopted for the solution of inverse shape reconstruction in acoustic scattering problems [34].

In this chapter we marry the level set approach with the Bayesian approach to geometric inverse problems. This leads to two significant advances: firstly it leads to a well-posed inverse problem in which the posterior distribution is Lipschitz with respect to the observed data, in the Hellinger metric – there is no analogous well-posedness theory for classical level set inversion; and secondly it leads to computationally expedient algorithms

in which the interfaces are updated implicitly via the Markov chain Monte Carlo (MCMC) methodology applied to the level set function – no explicit velocity field is required for the level set interface. We highlight that the recent paper [228] demonstrates the potential for working with regularised data misfit minimisation in terms of a level set function, but is non-Bayesian in its treatment of the problem, using instead simulated annealing within an optimisation framework. On the other hand the paper [231] adopts a Bayesian approach and employs the level set method, but requires a velocity field for propagation of the interface and does not have the conceptual and implementational simplicity, as well as the underlying theoretical basis, of the method introduced here. The papers [154, 155, 186], whilst motivated by the Bayesian approach, use the ensemble Kalman filter and are therefore not strictly Bayesian – the method does not deliver a provably reliable approximation of the posterior distribution except for linear Gaussian inverse problems.

The key idea which underpins our work is this. Both the theory and computational practice of the level set method for geometric inverse problems is potentially hampered by the fact that the mapping from the space of the level set function to the physical parameter space is discontinuous. This discontinuity occurs when the level set function is flat at the critical levels, and in particular where the desired level set has non-zero Lebesgue measure. This is dealt with in various *ad hoc* ways in the applied literature. The beauty of the Bayesian approach is that, with the right choice of prior in level set space, these discontinuities have probability zero. As a result a well-posedness theory (the posterior is Lipschitz in the data) follows automatically, and computational algorithms such as MCMC may be formulated in level set space. We thus have practical algorithms which are simultaneously founded on a sound theoretical bedrock.

In Section 6.2 we aim to build up a mathematical framework for Bayesian level set inversion. To do this, we first set up the inverse problem of interest in Section 6.2.1 where the unknown is an interface. To describe the geometry of the interface, a level set map is introduced in Section 6.2.2, whereby the inverse problem is reformulated in terms of a level set function which is thresholded to define the interfaces. Section 6.2.3 concerns the Bayesian approach to the inverse problem. Under certain assumptions on the negative log-likelihood function, it is shown that the posterior distribution exists and is stable with respect to perturbation of data; see the statements in Theorem 6.2.3. Since the well-posedness of the Bayesian inverse problem relies mostly on the almost sure continuity of the level set map, we discuss this issue thoroughly in Section 6.2.4. To be specific, we provide a complete characterisation for the discontinuity set of the level set map (in Proposition 6.2.6) and demonstrate the existence of Gaussian priors for which this discontinuity set is a probability zero event (in Proposition 6.2.8). In Section 6.3 we describe two examples – inverse gravimetry and permeability determination in groundwater flow – which

can be shown to satisfy the theoretical framework of the preceding section and hence for which there is a well-posed inverse problem for the level set function. Section 6.4 contains numerical experiments for both of these examples, demonstrating the potential of the methodology, and also highlighting important questions for future research. We conclude in Section 6.5, and then the two appendices contain various technical details and proofs which have been deferred in order to maintain the flow of ideas in the main body of the article.

6.2 Bayesian Level Set Inversion

6.2.1 The Inverse Problem

This chapter is concerned with inverse problems of the following type: recover function $\kappa \in X := L^q(D; \mathbf{R})$, D a bounded open set in \mathbf{R}^2 , from a finite set of noisily observed linear functionals $\{\mathcal{O}_j\}_{j=1}^J$ of $p \in V$, for some Banach space V , where $p = G(\kappa)$ for nonlinear operator $G \in C(X, V)$. Typically, for us, κ will represent input data for a partial differential equation (PDE), p the solution of the PDE and G the solution operator mapping the input κ to the solution p . Collecting the linear functionals into a single operator $\mathcal{O} : V \rightarrow \mathbf{R}^J$ and assuming additive noise $\eta \in \mathbf{R}^J$ we obtain the inverse problem of finding κ from y where

$$y = (\mathcal{O} \circ G)(\kappa) + \eta. \quad (6.1)$$

Since the composite mapping $\mathcal{O} \circ G$ is continuous from X to \mathbf{R}^J , identifying κ in the above under-determined inverse problem is well-adapted to both the classical [87] and Bayesian [61] approaches to regularised inversion. However interest is in geometric inverse problems using the level set formulation. For such problems, the mapping from the level set function to the data is discontinuous. Classical regularisation methods have problems in this situation; Example 6.2.1 below is an example of such a difficulty. However, we will demonstrate that formulating the inverse problem from the Bayesian point of view alleviates these issues and leads to a well-posed inverse problem.

6.2.2 Level Set Parameterisation

Assume that the physical parameter κ of the inverse problem is known *a priori* to have the form

$$\kappa(x) = \sum_{i=1}^n \kappa_i \mathbf{1}_{D_i}(x). \quad (6.2)$$

Here $\mathbf{1}_D$ denotes the indicator function of subset $D \subset \mathbf{R}^2$, $\{D_i\}_{i=1}^n$ are subsets of D such that $\bigcup_{i=1}^n \overline{D_i} = \overline{D}$ and $D_i \cap D_j = \emptyset$, and the $\{\kappa_i\}_{i=1}^n$ are known positive constants. Generalisation to the κ_i being unknown constants, or unknown smooth functions on each domain D_i , are possible but will not be considered explicitly in this chapter. Our focus is on the geometry of the interfaces implied by the D_i . In this setting the D_i become the primary unknowns and the level set method is natural. Given integer n fix the constants $c_i \in \mathbf{R}$ for $i = 0, \dots, n$ with $-\infty = c_0 < c_1 < \dots < c_n = \infty$ and consider a real-valued continuous level set function $u : D \rightarrow \mathbf{R}$. We can then define the D_i by

$$D_i = \{x \in D \mid c_{i-1} \leq u(x) < c_i\}. \quad (6.3)$$

It follows that $D_i \cap D_j = \emptyset$ for $i, j \geq 1$, $i \neq j$. For later use define the i -th level set $D_i^0 = \overline{D_i} \cap \overline{D_{i+1}} = \{x \in D \mid u(x) = c_i\}$. Let $U = C(\overline{D}; \mathbf{R})$ and, given the positive constants $\{\kappa_i\}_{i=1}^n$, we define the level set map $F : U \rightarrow X$ by

$$(Fu)(x) \rightarrow \kappa(x) = \sum_{i=1}^n \kappa_i \mathbf{1}_{D_i}(x). \quad (6.4)$$

We may now define $\mathcal{G} = \mathcal{O} \circ G \circ F : U \rightarrow \mathbf{R}^J$ and reformulate the inverse problem in terms of the level set function u : find u from y where

$$y = \mathcal{G}(u) + \eta. \quad (6.5)$$

However, because $F : U \rightarrow X$, and hence $\mathcal{G} : U \rightarrow \mathbf{R}^J$, is discontinuous, the classical regularisation theory for this form of inverse problem is problematic; this can be seen from the following example.

Example 6.2.1. Consider the inverse problem (6.5) where the level set map is given by the binary cut-off, i.e.

$$(Fu)(x) = \mathbf{1}_{u \geq 0}(x). \quad (6.6)$$

Classical regularisation methods seek the solution to the following minimisation problem:

$$\inf_{u \in E} I(u) := \inf_{u \in E} |y - \mathcal{G}(u)|^2 + \|u\|_E^p, \quad (6.7)$$

where E is some Banach space and $p \geq 1$. For instance, E could be a Sobolev space and $p = 2$ (Tikhonov-Phillips regularisation) or the space of functions of bounded variations and $p = 1$ (total variation regularisation). In the case of a Gaussian prior and an appropriate Sobolev norm, this variational problem will correspond to a maximum a posteriori

(MAP) estimator [136] and the analysis to follow shows a drawback of the MAP estimator in the context of level set thresholding.

Due to the discontinuity of F , we now show that the only possible minimiser of (6.7) is zero. In fact, suppose that $0 \neq \bar{u} \in E$ is a minimiser of I . We define $u_\varepsilon = \varepsilon \bar{u}$. Clearly u_ε and \bar{u} have the same zero level set when $\varepsilon > 0$. Then if $0 < \varepsilon < 1$,

$$|y - \mathcal{G}(\bar{u})|^2 = |y - \mathcal{G}(u_\varepsilon)|^2 \quad \text{and} \quad \|u_\varepsilon\|_E = \varepsilon \|\bar{u}\|_E, \quad (6.8)$$

which implies that $I(u_\varepsilon) < I(\bar{u})$ and hence contradicts with the assumption that \bar{u} is a minimiser. From (6.6), we see that the upper level set of the zero function is the whole domain, which does not provide any information about the geometry.

Whilst the current state of the art for Bayesian regularisation assumes continuity of \mathcal{G} for inverse problems of the form (6.5), we will demonstrate that the Bayesian setting can be generalised to level set inversion. This will be achieved by a careful understanding of the discontinuity set for F , and an understanding of probability measures for which this set is a measure zero event.

6.2.3 Well-Posed Bayesian Inverse Problem

We now formulate the Bayesian approach to finding u from y given by (6.5). All quantities are treated as random variables and we seek to find the posterior probability distribution on u given y , given a prior probability distribution on u and an independent probabilistic specification of the noise η . Let U denote a separable Banach space and define a complete probability space (U, Σ, μ_0) for the unknown u . Here Σ and μ_0 are the sigma algebra and prior probability measure, respectively. (In our applications U will be the space $C(\bar{D}; \mathbf{R})$ but we state our main theorem in more generality). Assume that the noise η is a random draw from the centred Gaussian $\mathbb{Q}_0 := N(0, \Gamma)$. Allowing for non-Gaussian η is also possible, as is dependence between η and u ; however we elect to keep the presentation simple. We may now define the joint random variable $(u, y) \in U \times \mathbf{R}^J$. The posterior probability distribution μ^y on the random variable $u|y$ describes our probabilistic knowledge about u on the basis of the measurements y given by (6.5) and the prior information μ_0 on u . In the case where the map \mathcal{G} is continuous, one can apply an infinite dimensional version of Bayes' theorem [215] to show that the posterior μ^y exists and has the density with respect to the prior of the form

$$\frac{d\mu^y}{d\mu_0}(u) = \frac{1}{Z} \exp(-\Phi(u; y)),$$

where Z is the normalisation constant. To extend the theory to allowing discontinuous \mathcal{G} , we now state a set of assumptions for the potential Φ , under which the posterior distribution

is well-defined via its density with respect to the prior distribution, and is Lipschitz in the Hellinger metric, with respect to data y . These assumptions will be verified for the level set formulation of interest to us.

Assumptions 6.2.2. *The function $\Phi : U \times \mathbf{R}^J \rightarrow \mathbf{R}$ and probability measure μ_0 on the measure space (U, Σ) satisfy the following properties:*

1. *for every $r > 0$ there is a $K = K(r)$ such that, for all $u \in U$ and all $y \in \mathbf{R}^J$ with $|y|_\Gamma < r$,*

$$0 \leq \Phi(u; y) \leq K;$$

2. *for any fixed $y \in \mathbf{R}^J$, $\Phi(\cdot; y) : U \rightarrow \mathbf{R}$, is continuous μ_0 -almost surely on the complete probability space (U, Σ, μ_0) ;*
3. *for $y_1, y_2 \in \mathbf{R}^J$ with $\max\{|y_1|_\Gamma, |y_2|_\Gamma\} < r$, there exists a $C = C(r)$ such that, for all $u \in U$,*

$$|\Phi(u; y_1) - \Phi(u; y_2)| \leq C|y_1 - y_2|_\Gamma.$$

For our Bayesian level set inverse problem with finite observations and noise $\eta \sim \mathbb{Q}_0$, the function $\Phi : U \times \mathbf{R}^J \rightarrow \mathbf{R}^+$ has the least squares form

$$\Phi(u; y) = \frac{1}{2}|y - \mathcal{G}(u)|_\Gamma^2 \tag{6.9}$$

with $|\cdot|_\Gamma := |\Gamma^{-\frac{1}{2}} \cdot|$ and $\mathcal{G} = \mathcal{O} \circ G \circ F$. Clearly Φ defined in (6.9) satisfies the first and the last item of Assumption 6.2.2. We will show in the next section that for some model problems, the second item of Assumption 6.2.2 will also be fulfilled by Φ in (6.9).

Recall that the Hellinger distance between μ and μ' is defined as

$$d_{\text{Hell}}(\mu, \mu') = \left(\frac{1}{2} \int_U \left(\sqrt{\frac{d\mu}{d\nu}} - \sqrt{\frac{d\mu'}{d\nu}} \right)^2 d\nu \right)^{\frac{1}{2}}$$

for any measure ν with respect to which μ and μ' are absolutely continuous. The Hellinger distance is, however, independent of which reference measure ν is chosen. We have the following:

Theorem 6.2.3. *Assume that the least squares function $\Phi : U \times \mathbf{R}^J \rightarrow \mathbf{R}$ given by (6.9) and the probability measure μ_0 on the measure space (U, Σ) satisfy Assumptions 6.2.2.*

Then $\mu^y \ll \mu_0$ with Radon-Nikodym derivative

$$\frac{d\mu^y}{d\mu_0} = \frac{1}{Z} \exp(-\Phi(u; y)) \quad (6.10)$$

where, for y almost surely,

$$Z := \int_U \exp(-\Phi(u; y)) \mu_0(du) > 0.$$

Furthermore μ^y is locally Lipschitz with respect to y , in the Hellinger distance: for all y, y' with $\max\{|y|_\Gamma, |y'|_\Gamma\} < r$, there exists a $C = C(r) > 0$ such that

$$d_{\text{Hell}}(\mu^y, \mu^{y'}) \leq C|y - y'|_\Gamma.$$

This implies that, for all $f \in L^2_{\mu_0}(U; S)$ for separable Banach space S ,

$$\|\mathbb{E}^{\mu^y} f(u) - \mathbb{E}^{\mu^{y'}} f(u)\|_S \leq C|y - y'|. \quad (6.11)$$

Remarks 6.2.4. • The interpretation of this result is very natural, linking the Bayesian picture with least squares minimisation: the posterior measure is large on sets where the least squares function is small, and vice-versa, all measured relative to the prior μ_0 .

- The key technical advance in this theorem over existing theories overviewed in [61] is that $\Phi(\cdot; y)$ is only continuous μ_0 -almost surely; existing theories typically use that $\Phi(\cdot; y)$ is continuous everywhere on U and that $\mu_0(U) = 1$; these existing theories cannot be used in the level set inverse problem, because of discontinuities in the level set map. Once the technical Lemma 6.6.1 has been established, which uses μ_0 -almost sure continuity to establish measurability, the proof of the theorem is a straightforward application of existing theory; we therefore defer it to Appendix 1.
- Stability estimates about the distance of level sets can be obtained by choosing f carefully in (6.11). Indeed, consider $f : U \mapsto L^1(D)$ given by

$$f(u)(x) := \mathbf{1}_{D_i}(x) \quad (6.12)$$

where D_i is defined in terms of u as in (6.3). Obviously $f \in L^2_{\mu_0}(U; L^1(D))$ since the indicator function is uniformly bounded. Then one can read from (6.11) that the L^1 -norm of mean indicator function of the set D_i under the posterior measure is Lipschitz continuous with respect to the data. Note that this does not give exactly the symmetric difference of the two mean level sets since indicator functions are averaged

first. However, it does reflect stability of geometric reconstructions in an averaged sense.

- What needs to be done to apply this theorem in our level set context is to identify the sets of discontinuity for the map \mathcal{G} , and hence $\Phi(\cdot; y)$, and then construct prior measures μ_0 for which these sets have measure zero. We study these questions in general terms in the next two subsections, and then, in the next section, demonstrate two test model PDE inverse problems where the general theory applies.
- The consequences of this result are wide-ranging, and we name the two primary ones: firstly we may apply the mesh-independent MCMC methods overviewed in [57] to sample the posterior distribution efficiently; and secondly the well-posedness gives desirable robustness which may be used to estimate the effect of other perturbations, such as approximating G by a numerical method, on the posterior distribution [61].

6.2.4 Discontinuity Sets of F

We return to the specific setting of the level set inverse problem where $U = C(\overline{D}; \mathbf{R})$. Consider the level set map $F : U \rightarrow L^q(D; \mathbf{R})$ with $1 \leq q \leq \infty$. First we note that it is not suitable to discuss the continuity of F by choosing $L^\infty(D, \mathbf{R})$ as the range space, simply because F could be discontinuous at very nice functions. We illustrate this point by means of the following elementary example.

Example 6.2.5. Let $U = C([-1, 1]; \mathbf{R})$ and define the level set map $F : U \mapsto L^\infty(-1, 1)$ by setting $F(u)(x) = \mathbf{1}_{\{u \geq 0\}}(x)$. Consider the linear function $u(x) = x$ and a sequence $u_n(x) = u(x) + 1/n$ for $n \in \mathbb{N}$. Clearly $u_n \rightarrow u$ in $C([-1, 1]; \mathbf{R})$. However, it is easy to see that $\|F(u_n) - F(u)\|_{L^\infty(-1, 1)} = 1 \not\rightarrow 0$.

However as a mapping $F : U \rightarrow L^q(D; \mathbf{R})$ for $q < \infty$ the situation is much better. Denoting by $m(A)$ the Lebesgue measure of a set $A \subset \mathbf{R}^2$, we have the following.

Proposition 6.2.6. For $u \in C(\overline{D})$ and $1 \leq q < \infty$, the level set map $F : C(\overline{D}) \rightarrow L^q(D)$ is continuous at u if and only if $m(D_i^0) = 0$ for all $i = 1, \dots, n-1$.

Remark 6.2.7. The fact that the continuity of level set map is related to the Lebesgue measure of the corresponding level sets has been observed already, see e.g. [99, Section 2.2]. However, we are not aware of any formal proof in the literature. Therefore we provide the complete proof below.

Proof of Proposition 6.2.6. “ \Leftarrow .” Let $\{u_\varepsilon\}$ denote any approximating family of level set functions with limit u as $\varepsilon \rightarrow 0$ in $C(\overline{D}; \mathbf{R}) : \|u_\varepsilon - u\|_{C(\overline{D})} < \varepsilon \rightarrow 0$. Let $D_{i,\varepsilon}, D_{i,\varepsilon}^0$ be

the sets defined in (6.3) associated with the approximating level set function u_ε and define $\kappa = F(u)$ by (6.4) and, similarly, $\kappa_\varepsilon := F(u_\varepsilon)$. Let $m(A)$ denote the Lebesgue measure of the set A .

Suppose that $m(D_i^0) = 0, i = 1, \dots, n-1$. Let $\{u_\varepsilon\}$ be the above approximating functions. We shall prove $\|\kappa_\varepsilon - \kappa\|_{L^q(D)} \rightarrow 0$. In fact, we can write

$$\begin{aligned}\kappa_\varepsilon(x) - \kappa(x) &= \sum_{i=1}^n \sum_{j=1}^n (\kappa_i - \kappa_j) \mathbf{1}_{D_{i,\varepsilon} \cap D_j}(x) \\ &= \sum_{i,j=1, i \neq j}^n (\kappa_i - \kappa_j) \mathbf{1}_{D_{i,\varepsilon} \cap D_j}(x).\end{aligned}$$

By the definition of u_ε , for any $x \in D$

$$u(x) - \varepsilon < u_\varepsilon(x) < u(x) + \varepsilon \quad (6.13)$$

Thus for $|j - i| > 1$ and ε sufficiently small, $D_{i,\varepsilon} \cap D_j = \emptyset$. For the case that $|i - j| = 1$, from (6.13), it is easy to verify that as $\varepsilon \rightarrow 0$,

$$\begin{aligned}D_{i,\varepsilon} \cap D_{i+1} &\subset \tilde{D}_{i,\varepsilon} := \{x \in D \mid c_i \leq u(x) < c_i + \varepsilon\} \rightarrow D_i^0, \quad i = 1, \dots, n-1, \\ D_{i,\varepsilon} \cap D_{i-1} &\subset \hat{D}_{i-1,\varepsilon} := \{x \in D \mid c_{i-1} - \varepsilon < u(x) < c_{i-1}\} \rightarrow \emptyset, \quad i = 2, \dots, n.\end{aligned} \quad (6.14)$$

By this and the assumption that $m(D_i^0) = 0$, we have that $m(D_{i,\varepsilon} \cap D_j) \rightarrow 0$ if $i \neq j$. Furthermore, the Lebesgue's dominated convergence theorem yields

$$\|\kappa_\varepsilon - \kappa\|_{L^q(D)}^q = \sum_{i,j=1, i \neq j}^n \int_{D_{i,\varepsilon} \cap D_j} |\kappa_i - \kappa_j|^q dx \rightarrow 0$$

as $\varepsilon \rightarrow 0$. Therefore, F is continuous at u .

“ \implies .” We prove this by contradiction. Suppose that there exists i^* such that $m(D_{i^*}^0) \neq 0$. We define $u_\varepsilon := u - \varepsilon$, then it is clear that $\|u_\varepsilon - u\|_{C(\overline{D})} \rightarrow 0$ as $\varepsilon \rightarrow 0$. By the same argument used in proving the sufficiency,

$$\begin{aligned}\|\kappa_\varepsilon - \kappa\|_{L^q(D)}^q &= \sum_{i=1}^{n-1} \int_{\tilde{D}_{i,\varepsilon} \cup \hat{D}_{i,\varepsilon}} |\kappa_{i+1} - \kappa_i|^q dx \\ &\rightarrow \sum_{i=1}^{n-1} \int_{D_i^0} |\kappa_{i+1} - \kappa_i|^q dx > \int_{D_{i^*}^0} |\kappa_{i^*+1} - \kappa_{i^*}|^q dx > 0\end{aligned}$$

where we have used $m(D_{i^*}^0) \neq 0$ in the last inequality. However, this contradicts with the assumption that F is continuous at u . \square

For the inverse gravimetry problem considered in the next section the space X is naturally $L^2(D; \mathbf{R})$ and we will be able to directly use the preceding proposition to establish the almost sure continuity of F and hence \mathcal{G} . For the groundwater flow inverse problem the space X is naturally $L^\infty(D; \mathbf{R})$ and we will not be able to use the proposition in this space to establish the almost sure continuity of F . However, we employ recent Lipschitz continuity results [22] for G on $L^q(D; \mathbf{R})$, $q < \infty$ to establish the almost sure continuity of \mathcal{G} .

6.2.5 Prior Gaussian Measures

Let D denote a bounded open subset of \mathbf{R}^2 . For our applications we will use the following two constructions of Gaussian prior measures μ_0 which are Gaussian $N(0, \mathcal{C}_i)$, $i = 1, 2$ on Hilbert function space \mathcal{H}_i , $i = 1, 2$.

- $N(0, \mathcal{C}_1)$ on

$$\mathcal{H}_1 := \{u : D \rightarrow \mathbf{R} \mid u \in L^2(D; \mathbf{R}), \int_D u(x) \, dx = 0\},$$

where

$$\mathcal{C}_1 = \mathcal{A}^{-\alpha} \quad \text{with } \alpha > 1 \text{ and } \mathcal{A} := -\Delta \quad (6.15)$$

with domain

$$D(\mathcal{A}) := \{u : D \rightarrow \mathbf{R} \mid u \in H^2(D; \mathbf{R}), \nabla u \cdot \nu = 0 \text{ on } \partial D \text{ and } \int_D u(x) \, dx = 0\}.$$

Here ν denotes the outward normal.

- $N(0, \mathcal{C}_2)$ on $\mathcal{H}_2 := L^2(D; \mathbf{R})$ with $\mathcal{C}_2 : \mathcal{H}_2 \rightarrow \mathcal{H}_2$ being the integral operator

$$\mathcal{C}_2 \phi(x) = \int_D c(x, y) \phi(y) \, dy \quad \text{with } c(x, y) = \exp\left(-\frac{|x - y|^2}{L^2}\right). \quad (6.16)$$

In fact, in the inverse model arising from groundwater flow studied in [125, 126], the Gaussian measure $N(0, \mathcal{C}_1)$ was taken as the prior measure for the logarithm of the permeability. On the other hand the Gaussian measure $N(0, \mathcal{C}_2)$ is widely used to model the earth's subsurface [177] as draws from this measure generate smooth random functions in which the parameter L sets the spatial correlation length. For both of these measures it is known that, under suitable conditions on the domain D , draws are almost surely in $C(\overline{D}; \mathbf{R})$; see [61, Theorems 2.16 and Theorem 2.18] for more details.

Since $\alpha > 1$ in (6.15), the Gaussian random function with measure μ_0 defined in either case above has the property that, for $U := C(\overline{D}; \mathbf{R})$, $\mu_0(U) = 1$. Since U is a separable Banach space μ_0 can be redefined as a Gaussian measure on U . Furthermore it is possible to define the appropriate σ -algebra Σ in such a way that (U, Σ, μ_0) is a complete probability space; for details see Appendix 2. We have the following, which is a subset of what is proved in Proposition 6.6.3.

Proposition 6.2.8. *Consider a random function u drawn from one of the Gaussian probability measures μ_0 on U given above. Then $m(D_i^0) = 0$, μ_0 -almost surely, for $i = 1, \dots, n$.*

□

This, combined with Proposition 6.2.6, is the key to making a rigorous well-posed formulation of Bayesian level set inversion. Together the results show that priors may be constructed for which the problematic discontinuities in the level set map are probability zero events. In the next section we demonstrate how the theory may be applied, by considering two examples.

6.3 Examples

6.3.1 Test Model 1 (Inverse Potential Problem)

Let $D \subset \mathbf{R}^2$ be a bounded open set with Lipschitz boundary. Consider the PDE

$$\Delta p = \kappa \quad \text{in } D, \quad p = 0 \quad \text{on } \partial D. \quad (6.17)$$

If $\kappa \in X := L^2(D)$ it follows that there is a unique solution $p \in H_0^1(D)$. Furthermore $\Delta p \in L^2(D)$, so that the Neumann trace can be defined in $V := H^{-\frac{1}{2}}(\partial D)$ by the following Green's formula:

$$\left\langle \frac{\partial p}{\partial \nu}, \varphi \right\rangle_{\partial D} = \int_D \Delta p \varphi \, dx + \int_D \nabla p \nabla \varphi \, dx$$

for $\varphi \in H^1(D)$. Here ν is the unit outward normal vector on ∂D and $\langle \cdot, \cdot \rangle_{\partial D}$ denotes the dual pairing on the boundary. We can then define the bounded linear map $G : X \rightarrow V$ by $G(\kappa) = \frac{\partial p}{\partial \nu}$.

Now assume that the source term κ has the form

$$\kappa(x) = \mathbf{1}_{D_1}(x)$$

for some $D_1 \subseteq D$. The inverse potential problem is to reconstruct the support D_1 from measurements of the Neumann data of p on ∂D . In the case where the Neumann data is

measured everywhere on the boundary ∂D , and where the domain D_1 is assumed to be star-shaped with respect to its centre of gravity, the inverse problem has a unique solution; see [129, 130] for details of this theory and see [37, 119] for discussion of numerical methods for this inverse problem. We will study the underdetermined case where a finite set of bounded linear functionals $\mathcal{O}_j : V \rightarrow \mathbf{R}$ are measured, noisily, on ∂D :

$$y_j = \mathcal{O}_j\left(\frac{\partial p}{\partial \nu}\right) + \eta_j. \quad (6.18)$$

Concatenating we have $y = (\mathcal{O} \circ G)(\kappa) + \eta$. Representing the boundary of D_1 as the zero level set of a function $u \in U := C(\overline{D}; \mathbf{R})$ we write the inverse problem in the form (6.5):

$$y = (\mathcal{O} \circ G \circ F)(u) + \eta. \quad (6.19)$$

Since multiplicity and uncertainty of solutions are then natural, we will adopt a Bayesian approach.

Notice that the level set map $F : U \rightarrow X$ is bounded: for all $u \in U$ we have $\|F(u)\|_X \leq \text{Vol}(D) := \int_D dx$. Since $G : X \rightarrow V$ and $\mathcal{O} : V \rightarrow \mathbf{R}^J$ are bounded linear maps it follows that $\mathcal{G} = \mathcal{O} \circ G \circ F : U \rightarrow \mathbf{R}^J$ is bounded: we have constant $C^+ \in \mathbf{R}^+$ such that, for all $u \in U$, $|\mathcal{G}(u)| \leq C^+$. From this fact Assumptions 6.2.2(1) and (3) follow automatically. Since both $G : X \rightarrow V$ and $\mathcal{O} : V \rightarrow \mathbf{R}^J$ are bounded, and hence continuous, linear maps, the discontinuity set of \mathcal{G} is determined by the discontinuity set of $F : U \rightarrow X$. By Proposition 6.2.6 this is precisely the set of functions for which the measure of the level set $\{u(x) = 0\}$ is zero. By Proposition 6.2.8 this occurs with probability zero for both of the Gaussian priors specified there and hence Assumptions 6.2.2(2) holds with these priors. Thus Theorem 6.2.3 applies and we have a well-posed Bayesian inverse problem for the level set function.

6.3.2 Test Model 2 (Discontinuity Detection in Groundwater Flow)

Consider the single-phase Darcy-flow model given by

$$-\nabla \cdot (\kappa \nabla p) = f \quad \text{in } D, \quad p = 0 \quad \text{on } \partial D. \quad (6.20)$$

Here D is a bounded Lipschitz domain in \mathbf{R}^2 , κ the real-valued isotropic permeability function and p the fluid pressure. The right hand side f accounts for the source of groundwater recharge. Let $V = H_0^1(D; \mathbf{R})$, $X = L^\infty(D; \mathbf{R})$ and V^* denote the dual space of V . If $f \in V^*$ and $X^+ := \{\kappa \in X : \text{essinf}_{x \in D} \kappa(x) \geq \kappa_{\min} > 0\}$ then $G : X^+ \mapsto V$ defined by

$G(\kappa) = p$ is Lipschitz continuous and

$$\|G(\kappa)\|_V = \|p\|_V \leq \|f\|_{V^*} / \kappa_{\min}. \quad (6.21)$$

We consider the practically useful situation in which the permeability function κ is modelled as piecewise constant on different regions $\{D_i\}_{i=1}^n$ whose union comprise D ; this is a natural way to characterise heterogeneous subsurface structure in a physically meaningful way. We thus have

$$\kappa(x) = \sum_{i=1}^n \kappa_i \mathbf{1}_{D_i}(x)$$

where $\{D_i\}_{i=1}^n$ are subsets of D such that $\cup_{i=1}^n \overline{D_i} = \overline{D}$ and $D_i \cap D_j = \emptyset$, and where the $\{\kappa_i\}_{i=1}^n$ are positive constants. We let $\kappa_{\min} = \min_i \kappa_i$.

Unique reconstruction of the permeability in some situations is possible if the pressure p is measured everywhere [4, 196]. The inverse problem of interest to us is to locate the discontinuity set of the permeability from a finite set of measurements of the pressure p . Such problems have also been studied in the literature. For instance, the paper [218] considers the problem by using multiple level set methods in the framework of optimisation; and in [127], the authors adopt a Bayesian approach to reconstruct the permeability function characterised by layered or channelized structures whose geometry can be parameterised finite dimensionally. As we consider a finite set of noisy measurements of the pressure p , in V^* , and the problem is underdetermined and uncertain, the Bayesian approach is again natural. We make the significant extension of [127] to consider arbitrary interfaces, requiring infinite dimensional parameterisation: we introduce a level set parameterisation of the domains D_i , as in (6.3) and (6.4).

Let $\mathcal{O} : V \rightarrow \mathbf{R}^J$ denote the collection of J linear functionals on V which are our measurements. Because of the estimate (6.21) it is straightforward to see that $\mathcal{G} = \mathcal{O} \circ G \circ F$ is bounded as a mapping from U into \mathbf{R}^J and hence that Assumptions 6.2.2(1) and (3) hold; it remains to establish (2). To that end, from now on we need slightly higher regularity on f . In particular, we assume that, for some $q > 2$, $f \in W^{-1}(L^q(D))$. Here the space $W^{-1}(L^q(D)) := (W_0^{1,q^*}(D))^* \subset V^*$ for q^* and q conjugate: $1/q + 1/q^* = 1$. It is shown in [22] that there exists $q_0 > 2$ such that the solution of (6.20) satisfies

$$\|\nabla p\|_{L^q(D)} \leq C \|f\|_{W^{-1}(L^q(D))}$$

for some $C < \infty$ provided $2 \leq q < q_0$. We assume that such a q is chosen. It then follows that G is Lipschitz continuous from L^r to V where $r := 2q/(q-2) \in [2, \infty)$. To be precise,

let p_i be the solution to the problem (6.20) with $\kappa_i, i = 1, 2$. Then the following is proved in [22]: for any $q \geq 2$,

$$\|p_1 - p_2\|_V \leq \frac{1}{\kappa_{\min}} \|\nabla p_1\|_{L^q(D)} \|\kappa_1 - \kappa_2\|_{L^r(D)}$$

provided $\nabla p_1 \in L^q(D)$.

Hence $G : L^r(D) \rightarrow V$ is Lipschitz under our assumption that $f \in W^{-1}(L^q(D))$ for some $q \in (2, \infty)$. By viewing $F : U \rightarrow L^r(D)$, it follows from Proposition (6.2.6) and Proposition (6.2.8) that Assumptions (6.2.2) (2) holds with both Gaussian priors defined in Section 6.2.5. As a consequence Theorem 6.2.3 also applies in the groundwater flow model.

6.4 Numerical Experiments

Application of the theory developed in Section 6.2.3 ensures that, for the choices of Gaussian priors discussed in Section 6.2.5, the posterior measure on the level set is well defined and thus suitable for numerical interrogation. In this section we display numerical experiments where we characterise the posterior measure by means of sampling with MCMC. In concrete we apply the preconditioned Crank-Nicolson MCMC (pCN-MCMC) method explained in [57]. We start by defining this algorithm. Assume that we have a prior Gaussian measure $N(0, \mathcal{C})$ on the level set function u and a posterior measure μ^y given by (6.10). Define

$$a(u, v) = \min\{1, \exp(\Phi(u) - \Phi(v))\}$$

and generate $\{u^{(k)}\}_{k \geq 0}$ as follows:

Algorithm 6.4.1 (pCN-MCMC).

Set $k = 0$ and pick $u^{(0)} \in X$.

1. *Propose $v^{(k)} = \sqrt{(1 - \beta^2)}u^{(k)} + \beta\xi^{(k)}$, $\xi^{(k)} \sim N(0, \mathcal{C})$.*
2. *Set $u^{(k+1)} = v^{(k)}$ with probability $a(u^{(k)}, v^{(k)})$, independently of $(u^{(k)}, \xi^{(k)})$.*
3. *Set $u^{(k+1)} = u^{(k)}$ otherwise.*
4. *$k \rightarrow k + 1$ and return to 1.*

Then the resulting Markov chain is reversible with respect to μ^y and, provided it is ergodic, satisfies

$$\frac{1}{K} \sum_{k=0}^K \varphi(u^{(k)}) \rightarrow \mathbb{E}^{\mu^y} \varphi(u)$$

for any test function φ with suitable regularity. Furthermore a central limit theorem determines the fluctuations around the limit, which are asymptotically of size $K^{-\frac{1}{2}}$.

6.4.1 Aim of The Experiments

By means of the MCMC method described above we explore the Bayesian posterior of the level set function that we use to parametrise unknown geometry (or discontinuous model parameters) in the geometric inverse problems discussed in Section 6.3. The first experiment of this section concerns the inverse potential problem defined in Section 6.3.1. The second and third experiments are concerned with the estimation of geologic facies for the groundwater flow model discussed in Section 6.3.2. The main objective of these experiments is to display the capabilities of the level set Bayesian framework to provide an estimate, along with a measure of its uncertainty, of unknown discontinuous model parameters in these test models. We recall that for the inverse potential problem the aim is to estimate the support D_1 of the indicator function $\kappa(x) = \mathbf{1}_{D_1}(x)$, that defines the source term of the PDE (6.17), given data/observations from the solution of this PDE. Similarly, given data/observations from the solution of the Darcy flow model (6.20), we wish to estimate the interface between geologic facies $\{D_i\}_{i=1}^n$ corresponding to regions of different structural geology and which leads to a discontinuous permeability $\kappa(x) = \sum_{i=1}^n \kappa_i \mathbf{1}_{D_i}(x)$ in the flow model (6.20). In both test models, we introduce the level set function merely as an artefact to parametrise the unknown geometry (i.e. $D_i = \{x \in D \mid c_{i-1} \leq u(x) < c_i\}$), or equivalently, the resulting discontinuous field $\kappa(x)$. The Bayesian framework applied to this level-set parametrisation then provides us with a posterior measure μ^y on the level set function u . The push-forward of μ^y under the level set map F (6.4) results in a distribution on the discontinuous field of interest κ . This push-forward of the level set posterior $F^* \mu^y := \mu^y \circ F^{-1}$ comprises the statistical solution of the inverse problem which may, in turn, be used for practical applications.

A secondary aim of the experiments is to explore the role of the choice of prior on the posterior. Because the prior is placed on the level set function, and not on the model parameters of direct interest, this is a non-trivial question. To be concrete, the posterior depends on the Gaussian prior that we put on the level set. While the prior may incorporate our a priori knowledge concerning the regularity and the spatial correlation of the unknown geometry (or alternatively, the regions of discontinuities in the fields of interest) it is clear that such selection of the prior on the level set may have a strong effect on the resulting posterior μ^y and the corresponding push-forward $F^* \mu^y$. One of the key aspects of the subsequent numerical study is to understand the role of the selection of the prior on the level set functions in terms of the quality and efficiency of the solution to the Bayesian inverse problem as expressed via the push-forward of the posterior $F^* \mu^y$.

6.4.2 Implementational Aspects

For the numerical examples of this section we consider synthetic experiments. The PDEs that define the forward models of Section 6.3 (i.e. expressions (6.17) and (6.20)) are solved numerically, on the unit-square, with cell-centred finite differences [7]. In order to avoid inverse crimes [136], for the generation of synthetic data we use a much finer grid (size specified below) than the one of size 80×80 used for the inversion via the MCMC method displayed in Algorithm 6.4.1.

Algorithm 6.4.1 requires, in step (i), sampling of the prior. This is accomplished by parameterising the level set function in terms of the Karhunen-Loève (KL) expansion associated to the prior covariance operator \mathcal{C} (See Appendix 2, equation (6.24)). For the purpose of numerics, the infinite series of the KL expansion is truncated; theoretical results concerning the effect of this finite dimensional approximation on the posterior can be found in [58]. Upon discretisation, the number of eigenvectors of \mathcal{C} equals the dimensions of the discretised physical domain of the model problems (i.e. $N = 6400$ in expression (6.25)). Once the eigen-decomposition of \mathcal{C} has been conducted, then sampling from the prior can be done simply by sampling an i.i.d set of random variables $\{\xi_k\}$ with $\xi_1 \sim N(0, 1)$ and using it in (6.25). During the burn-in period (which here is taken to comprise 10^4 iterations) of the MCMC method, we find it advantageous to freeze the higher KL modes and conduct the sampling only for the lower modes. After the aforementioned burn-in, the sampling is then carried out on the full set of KL modes represented on the given computational mesh. This freezing of modes during the burn-in enables the MCMC method to quickly reach an “optimal” state where the samples of the level set function provide fields $\kappa(x)$ that are close to the truth. However, once this optimal state has been reached, it is essential to conduct the sampling on the full spectrum of KL modes to ensure that the MCMC chain mixes and properly represents the posterior uncertainty. More precisely, if only the lowest modes are retained for the full chain, the MCMC may collapse into the optimal state but without mixing. Thus, while the lowest KL modes determine the main geometric structure of the underlying discontinuous field, the highest modes are essential for the proper mixing and thus the proper and efficient characterisation of the posterior.

6.4.3 Inverse Potential Problem

In this experiment we generate synthetic data by solving (6.17), on a fine grid of size 240×240 with the “true” indicator function $\kappa^\dagger = \mathbf{1}_{D_1^\dagger}$ displayed in Figure 6.1 (top). The observation operator $\mathcal{O} = (\mathcal{O}_1, \dots, \mathcal{O}_{64})$ is defined in terms of 64 mollified Dirac deltas $\{\mathcal{O}_j\}_{j=1}^{64}$ centred at the measurement locations display as white squares along the boundary of the domain in Figure 6.1 (top). Each coordinate of the data is computed by means

of (6.19) with p from the solution of the PDE with the aforementioned true source term and by adding Gaussian noise η_j with standard deviation of 10% of the size of the noise-free measurements (i.e. of $\mathcal{O}_j(\frac{\partial p}{\partial \nu})$). We reiterate that, in order to avoid inverse crimes [136], we use a coarser grid of size 80×80 for the inversion via the MCMC method (Algorithm 6.4.1). The parametrisation of D_1 in terms of the level set function is given by $D_1 = \{x \in D \mid u(x) < 0\}$ (i.e. by simply choosing $c_0 = -\infty$ and $c_1 = 0$ in (6.3)).

For this example we consider a prior covariance \mathcal{C} of the form presented in (6.16) for some choices of L in the correlation function. We construct \mathcal{C} directly from this correlation function and then we conduct the eigen-decomposition needed for the KL expansion and thus for sampling the prior. In Figure 6.2 we display samples from the prior $N(0, \mathcal{C})$ on the level set function u (first, third and fifth rows) and the corresponding indicator function $\kappa = \mathbf{1}_{D_1}$ (second, fourth and sixth rows) for (from left to right) $L = 0.1, 0.15, 0.2, 0.3, 0.4$. Different values of L in (6.16) clearly result in substantial differences in the spatial correlation of the zero level set associated to the samples of the level set function. The spatial correlation of the zero level set function, under the prior, has significant effect on $\mathbf{1}_{D_1}$ which we use as the right-hand side (RHS) in problem (6.17) and whose solution, via expression (6.19), determines the likelihood (6.9). It then comes as no surprise that the posterior measure on the level set is also strongly dependent on the choice of the prior via the parameter L . We explore this effect in the following paragraphs.

In Figure 6.3 we present the numerical results from different MCMC chains computed with different priors corresponding to the aforementioned choices of L . The MCMC mean of the level set function is displayed in the top row of Figure 6.3 for the choices (from left to right) $L = 0.1, 0.15, 0.2, 0.3, 0.4$. We reiterate that although the MCMC method provides the characterisation of the posterior of the level set function, our primary aim is to identify the field $\kappa(x) = \mathbf{1}_{D_1}(x)$ that determines the RHS of (6.17) by means of conditioning the prior $N(0, \mathcal{C})$ to noisy data from (6.19). A straightforward estimate of such field can be obtained by mapping, via the level set map (6.4), the posterior mean level set function denoted by \bar{u} into the corresponding field $F(\bar{u}(x)) = \bar{\kappa}(x) = \mathbf{1}_{\bar{D}_1}(x)$ where $\bar{D}_1 = \{x \in D \mid \bar{u}(x) < 0\}$. We display $\bar{\kappa}(x) = \mathbf{1}_{\bar{D}_1}(x)$ in the top-middle row of Figure 6.3 along with the plot of the true field $\kappa^\dagger = \mathbf{1}_{D_1^\dagger}$ (right column) for comparison.

As mentioned earlier, we are additionally interested in the push-forward of the posterior measure of the level set function u under the level set map (i.e. $(F^* \mu^y)(du)$). We characterise $F^* \mu^y$ by mapping under F our MCMC samples from μ^y . In Figure 6.3 we present the mean (bottom-middle) and the variance (bottom) of $F^* \mu^y$. Figure 6.4 shows some posterior (MCMC) samples u of the level set function (first, third and fifth rows) and the corresponding level set map $F(u) = \mathbf{1}_{D_1}$ with $D_1 = \{x \in D \mid u(x) < 0\}$ associated to these posterior samples (second, fourth and sixth rows).

The push-forward of the posterior measure under the level set map (i.e. $F^*\mu^y$) thus provides a probabilistic description of the inverse problem of identifying the true $\kappa^\dagger = \mathbf{1}_{D_1^\dagger}$. We can see from Figure 6.3 that, for some choices of L , the mean of $F^*\mu^y$ provides reasonable estimates of the truth. However, the main advantage of the Bayesian approach proposed here is that a measure of the uncertainty of such estimate is also obtained from $F^*\mu^y$. The variance (Figure 6.3 bottom), for example, is a measure of the uncertainty in the location of the interface between the two regions D and $D \setminus D_1$.

The results displayed in Figure 6.3 show the strong effect that the selection of the prior has on the posterior measure μ^y and the corresponding push-forward measure $F^*\mu^y$. In particular, there seems to be a critical value $L = 0.2$ above of which the corresponding posterior mean on $F^*\mu^y$ provides a reasonable identification of the true $\mathbf{1}_{D_1^\dagger}$ with relatively small variance. This critical value seems to be related to the size and the shape of the inclusions that determines the true region D_1^\dagger (Figure 6.1 (top)). It is intuitive that posterior samples that result from very small spatial correlation cannot easily characterise these inclusions accurately unless the data is overwhelmingly informative. The lack of a proper characterisation of the geometry from priors associated with small L is also reflected with larger variance around the interface. It is then clear that the capability of the proposed level set Bayesian framework to properly identify a shape D_1^\dagger (or alternatively its indicator function $\mathbf{1}_{D_1^\dagger}$) depends on properly incorporating, via the prior measure, a priori information on the regularity and spatial correlation of the unknown geometry of D_1^\dagger .

Since the selection of the prior has such a clear effect on the posterior, it comes as no surprise that it also affects the efficiency of the MCMC method as we now discuss. In the bottom-right panel of Figure 6.1 we show the autocorrelation function (ACF, see [31]) of the first KL mode of the level set function from different MCMC chains with different priors corresponding to our different choices of correlation length L in (6.16). The tunable parameters in the pCN-MCMC method are fixed for these experiments. We recall from Figure 6.3 that larger values of L result in a mean level set whose corresponding indicator function better captures the spatial structures from the truth and with smaller variance around the interface. However, the larger the value of L the slower the decay of the ACF. From these ACF plots, we note that even for the apparent optimal value of $L = 0.3$, our MCMC method produces samples that are highly correlated and thus very long chains may be needed in order to produce a reasonable number of uncorrelated samples needed for statistical analysis. For this particular choice of $L = 0.3$ we have conducted 50 multiple MCMC chains of length 10^6 (after burn-in period) initialised from random samples from the prior. In Figure 6.1 (bottom-left) we show the potential scale reduction factor (PSRF, see [32] for a definition) computed from MCMC samples of the level set function (red-solid line) and the corresponding samples under F (i.e. the $\mathbf{1}_{D_1}$'s) (blue-dotted line) which

corresponds to the RHS of (6.17). We observe that the PSRF goes below 1.1 after (often taken as an approximate indication of convergence [32]); thus the Gelman-Rubin diagnostic [32] based on the PSRF is passed for this selection of L . The generation of multiple independent MCMC chains that are statistically consistent opens up the possibility of using high-performance computing to enhance our capabilities of properly exploring the posterior. While we use a relatively small number of chains as a proof-of-concept, the MCMC chains are fully independent and so the computational cost of running multiple chains scales with the number of available processors.

The 5×10^7 samples that we obtained from the 50 MCMC chains are combined to provide a full characterisation of the posterior μ^y on the level set and the corresponding push-forward $F^*\mu^y$ (i.e. The $\mathbf{1}_{D_1}$'s computed from D_1 with posterior samples u). We reemphasise that our aim is the statistical identification of $\mathbf{1}_{D_1^\dagger}$. Therefore, in order to obtain a quantity from the true $\mathbf{1}_{D_1^\dagger}$ against to which compare the computed push-forward of the level set posterior, we consider the Discrete Cosine Transform (DCT) of the true field $\mathbf{1}_D$. Other representations/expansions of the true field could be considered for the sake of assessing the uncertainty of our estimates with respect to the truth. In Figure 6.5 we show the prior and posterior densities of the first DCT coefficients of $\mathbf{1}_{D_1}$ where $D_1 = \{x \in D \mid u(x) < 0\}$ with u from our MCMC samples (the vertical dotted line corresponds to the DCT coefficient of the true $\mathbf{1}_{D_1^\dagger}$). We can observe how the push forward posterior are concentrated around the true values. It is then clear how the data provide a strong conditioning on the first DCT coefficients of the discontinuous field that we aim at obtaining with our Bayesian level set approach.

While the main objective of our Bayesian methodology is to characterise the posterior, it is relevant to assess the accuracy of this methodology at approximating the truth κ^\dagger . To this end we define the following L^1 -relative error:

$$\mathcal{E}_{L^1}(\xi) \equiv \frac{\|\xi - \kappa^\dagger\|_{L^1(D)}}{\|\kappa^\dagger\|_{L^1(D)}}. \quad (6.22)$$

In Figure 6.6 (left) we plot $\mathcal{E}_{L^1}(F(\bar{u}_n))$ which corresponds to the relative error with respect to the truth κ^\dagger , at the n th MCMC iteration, of the MCMC sample mean \bar{u}_n under the map F . Figure 6.6 (middle) displays $\mathcal{E}_{L^1}(\bar{\kappa}_n)$, i.e. the error of the sample mean of the push-forward samples under F (i.e. the mean of the samples $\kappa_n = F(u_n)$). Finally, in Figure 6.6 (right) we show $\mathcal{E}_{L^1}(F(u_n))$, the error of the push-forward under F of the n th MCMC sample. We can clearly appreciate that the most accurate results corresponds to $L = 0.3$ and $L = 0.4$ which are, in turn, the cases with less uncertainty in terms of the variance (see Figure 6.3 bottom row). The larger size of the errors in the rightmost panel is a reflection of the uncertainty in the reconstruction, and the posterior variance in the estimates.

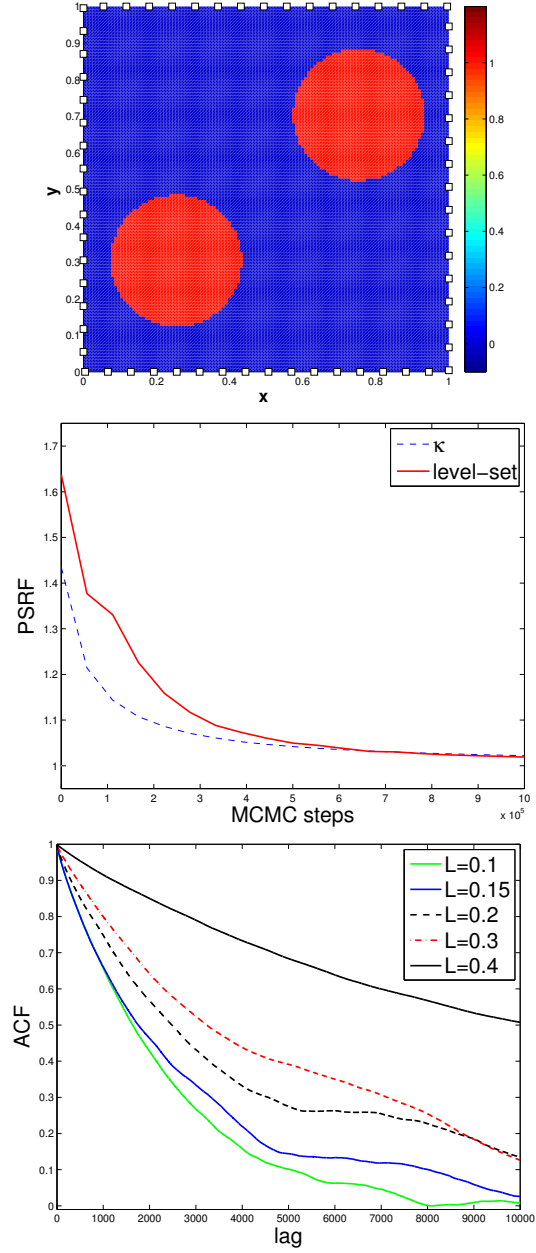


Figure 6.1: Inverse Potential. Top: True source term $\kappa^\dagger = \mathbf{1}_{D_1^\dagger}$ of eq. (6.17). Bottom-left: PSRF from multiple chains with $L = 0.3$ in (6.16). The PSRF is computed from level-set samples (solid red line) as well as the corresponding $\kappa = \mathbf{1}_{D_1}$ (blue dotted line). Bottom-right: ACF of first KL mode of the level set function from single-chain MCMC with different choices of L .

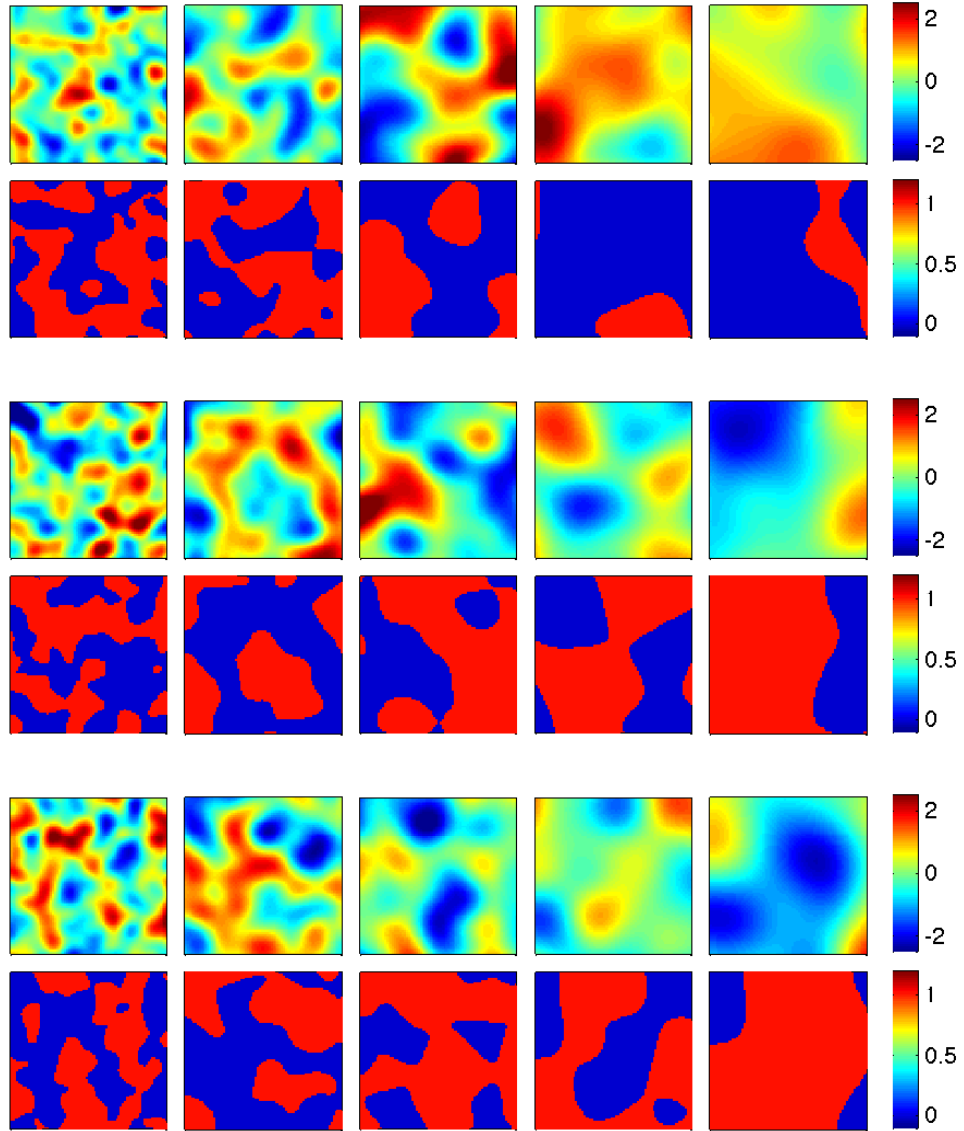


Figure 6.2: Inverse Potential. Samples from the prior on the level set function u (first, third and fifth rows) for (from left to right) $L = 0.1, 0.15, 0.2, 0.3, 0.4$. Corresponding 1_{D_1} with $D_1 = \{x \in D \mid u(x) < 0\}$ (second, fourth and sixth rows) associated to each of these samples from the level set function.

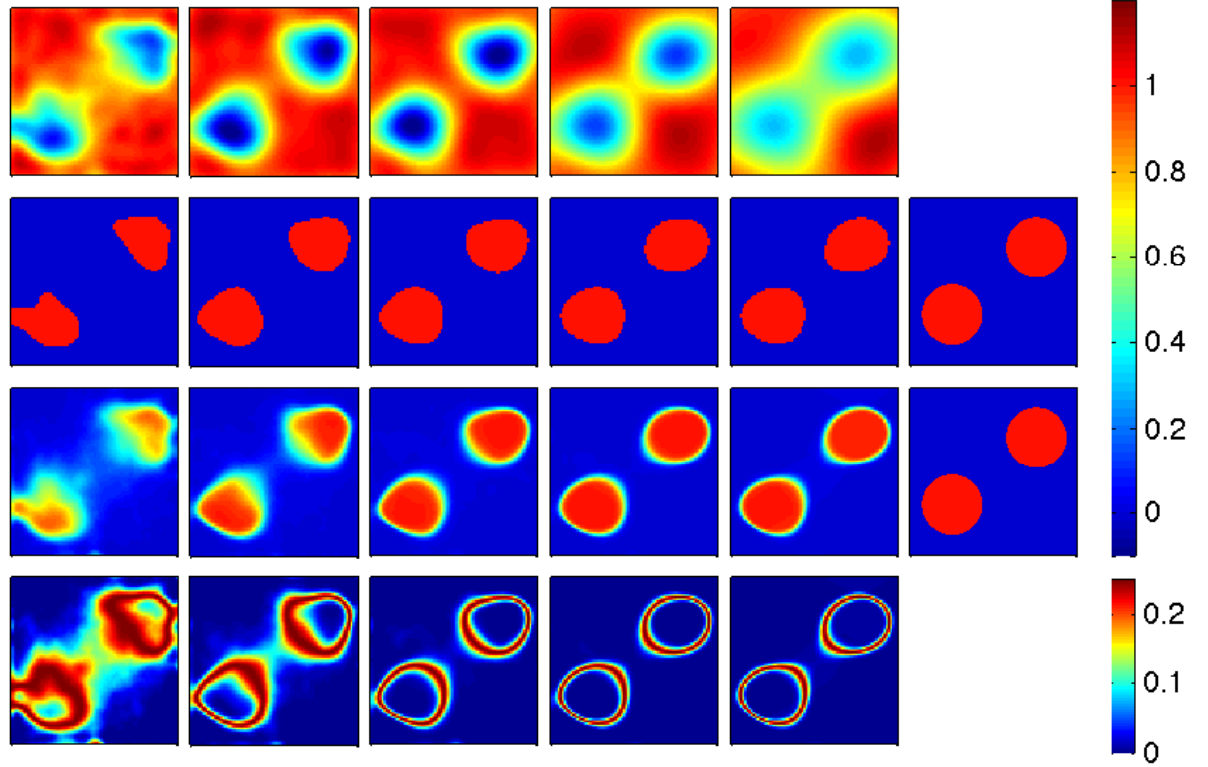


Figure 6.3: Inverse Potential. MCMC results for (from left to right) $L = 0.1, 0.15, 0.2, 0.3, 0.4$ in the eq. (6.16). Top: Posterior mean level set function \bar{u} (computed via MCMC). Top-middle: Plot of $\mathbf{1}_{\bar{D}_1}$ with $\bar{D}_1 = \{x \in D \mid \bar{u}(x) < 0\}$ (the truth $\mathbf{1}_{D_1^\dagger}$ is presented in the right column). Bottom-middle: Mean of $\mathbf{1}_{D_1}$ where $D_1 = \{x \in D \mid u(x) < 0\}$ and u 's are the posterior MCMC samples (the truth is presented in the right column). Bottom: Variance of $\mathbf{1}_{D_1}$ where $D_1 = \{x \in D \mid u(x) < 0\}$ and u 's are the posterior MCMC samples

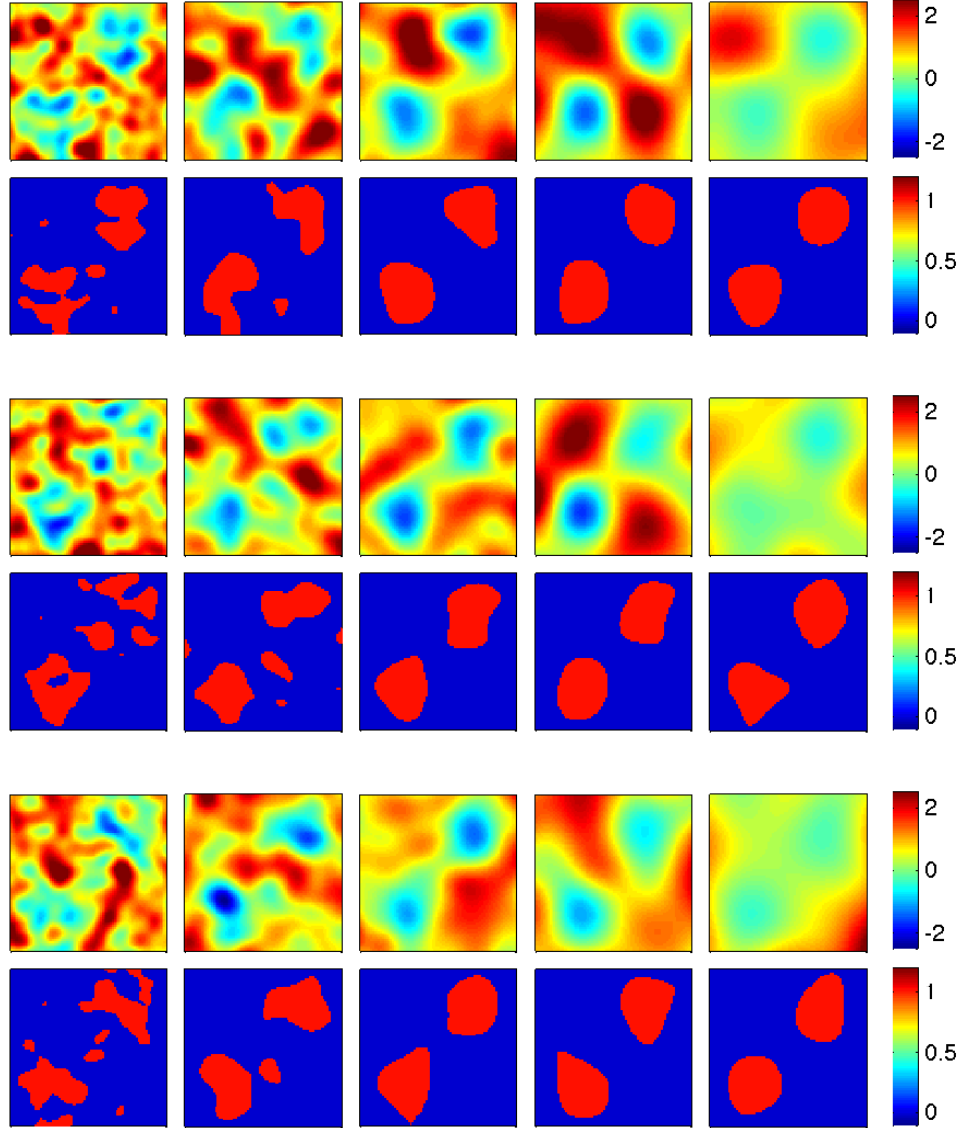


Figure 6.4: Inverse Potential. Samples from the posterior on the level set u (first, third and fifth rows) for (from left to right) $L = 0.1, 0.15, 0.2, 0.3, 0.4$. Corresponding $\mathbf{1}_{D_1}$ where $D_1 = \{x \in D \mid u(x) < 0\}$ (second, fourth and sixth rows) associated to each of these samples from the level set function.

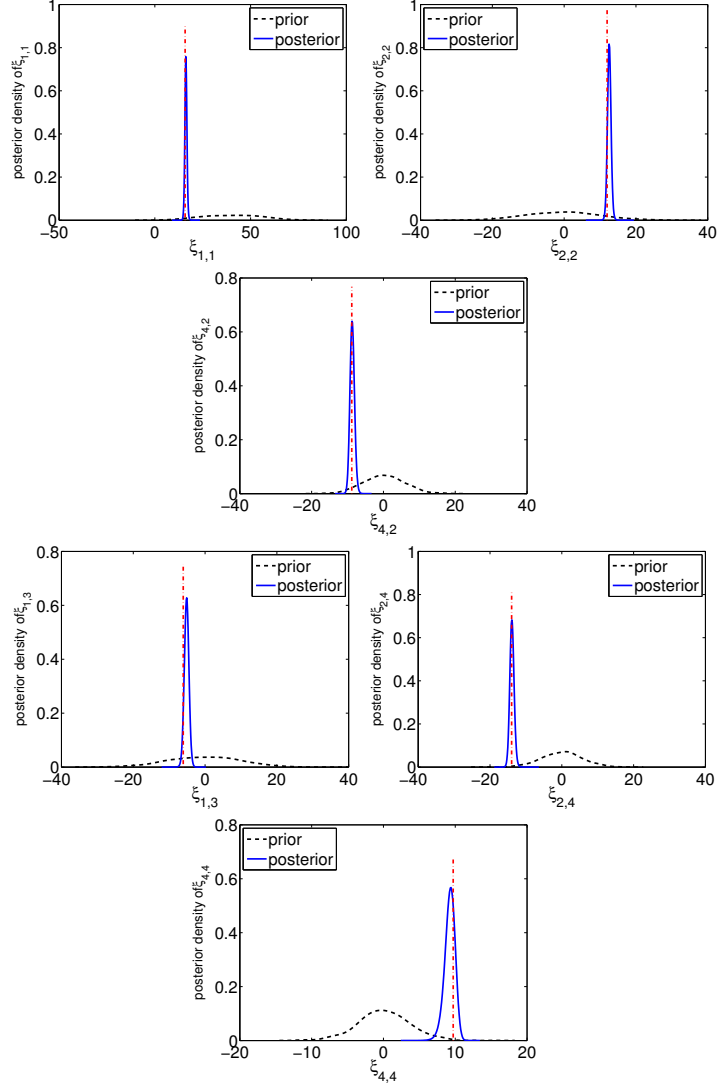


Figure 6.5: Inverse Potential. Densities of the prior and posterior of various DCT coefficients of the $\mathbf{1}_{D_1}$ where $D_1 = \{x \in D \mid u(x) < 0\}$ obtained from MCMC samples on the level set u for $L = 0.3$ (vertical dotted line indicates the truth).

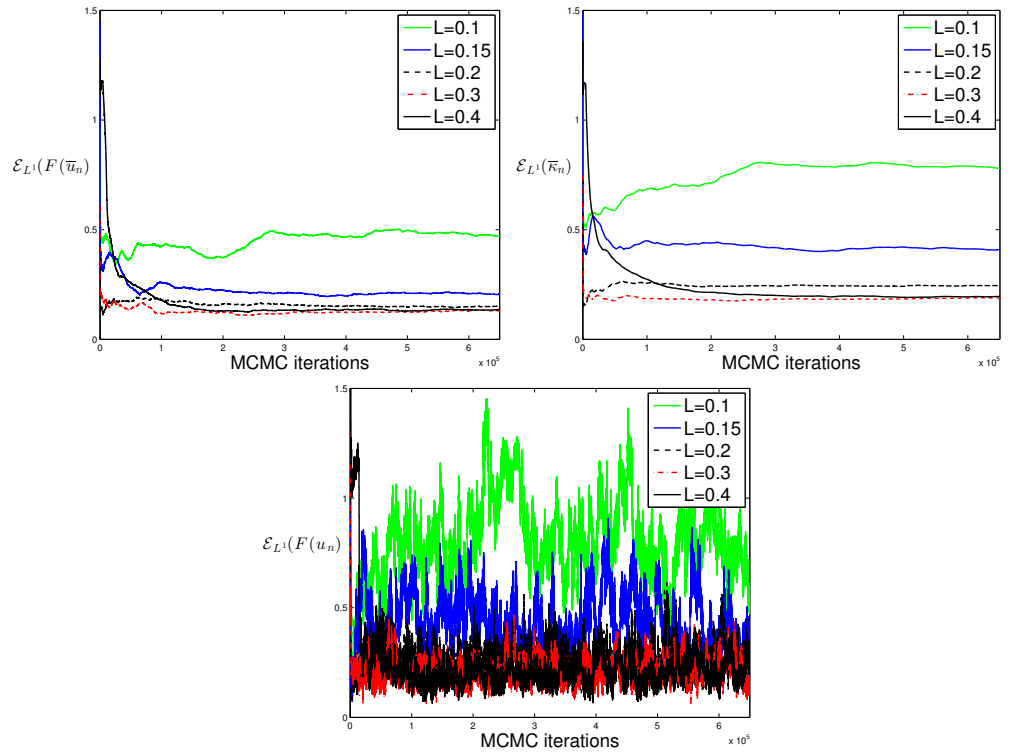


Figure 6.6: Inverse Potential. $L^1(D)$ relative errors with respect to the truth for different choices of L . Left: $\mathcal{E}_{L^1}(F(\bar{u}_n))$. Middle: $\mathcal{E}_{L^1}(\bar{\kappa}_n)$. Right: $\mathcal{E}_{L^1}(F(u_n))$

6.4.4 Structural Geology: Channel Model

In this section we consider the inverse problem discussed in Section 6.3.2. We consider the Darcy model (6.20) but with a more realistic set of boundary conditions that consist of a mixed Neumann and Dirichlet conditions. For the concrete set of boundary conditions as well as the right-hand-side we use for the present example we refer the reader to [125, Section 4]. This flow model, initially used in the seminal paper of [45], has been used as a benchmark for inverse problems in [113, 124, 125]. While the mathematical analysis of subsection 6.3.2 is conducted on a model with Dirichlet boundary conditions, in order to streamline the presentation, the corresponding extension to the case of mixed boundary conditions can be carried out with similar techniques.

We recall that the aim is to estimate the interface between regions D_i of different structural geology which result in a discontinuous permeability κ of the form (6.2). In order to generate synthetic data, we consider a true $\kappa^\dagger(x) = \sum_{i=1}^3 \kappa_i \mathbf{1}_{D_i^\dagger}$ with prescribed (known) values of $\kappa_1 = 7$, $\kappa_2 = 50$ and $\kappa_3 = 500$. This permeability, whose plot is displayed in Figure 6.7 (top), is used in (6.20) to generate synthetic data collected from interior measurement locations (white squares in Figure 6.7). The estimation of κ is conducted given observations of the solution of the Darcy model (6.20). To be concrete, the observation operator $\mathcal{O} = (\mathcal{O}_1, \dots, \mathcal{O}_{25})$ is defined in terms of 25 mollified Dirac deltas $\{\mathcal{O}_j\}_{j=1}^{25}$ centred at the aforementioned measurement locations and acting on the solution p of the Darcy flow model. For the generation of synthetic data we use a grid of 160×160 which, in order to avoid inverse crimes [136], is finer than the one used for the inversion (80×80). As before, observations are corrupted with Gaussian noise proportional to the size of the noise-free observations ($\mathcal{O}_j(p)$ in this case).

For the estimation of κ with the proposed Bayesian framework we assume that knowledge of three nested regions is available with the permeability values $\{\kappa_i\}_{i=1}^3$ that we use to define the true κ^\dagger . Again, we are interested in the realistic case where the rock types of the formation are known from geologic data but the location of the interface between these rocks is uncertain. In other words, the unknowns are the geologic facies D_i that we parametrise in terms of a level set function, i.e. $D_i = \{x \in D \mid c_{i-1} \leq u(x) < c_i\}$ with $c_0 = -\infty$, $c_1 = 0$, $c_2 = 1$, $c_3 = \infty$. Similar to the previous example, we use a prior of the form (6.16) for the level set function. In Figure 6.8 we display samples from the prior on the level set function (first, third and fifth rows) and the corresponding permeability mapping under the level set map (6.4) $F(u)(x) = \kappa(x) = \sum_{i=1}^3 \kappa_i \mathbf{1}_{D_i}$ (second, fourth and sixth rows) for (from left to right) $L = 0.2, 0.3, 0.35, 0.4, 0.5$. As before, we note that the spatial correlation of the covariance function has a significant effect on the spatial correlation of the interface between the regions that define the interface between the geologic facies (alternatively, the discontinuities of κ). Longer values of L provide

κ 's that seem more visually consistent with the truth. The results from Figure 6.9 show MCMC results from experiments with different priors corresponding to the aforementioned choices of L . The posterior mean level set function \bar{u} is displayed in the top row of Figure 6.9. The corresponding mapping under the level set function $\bar{\kappa} \equiv \sum_{i=1}^3 \kappa_i \mathbf{1}_{\bar{D}_i}$ (with $\bar{D}_i = \{x \in D \mid c_{i-1} \leq \bar{u}(x) < c_i\}$) is shown in the top-middle.

Similar to our discussion of the preceding subsection, for the present example we are interested in the push-forward of the posterior μ^y under the level set map F . More precisely, $F^* \mu^y$ provides a probability description of the solution to the inverse problem of finding the permeability given observations from the Darcy flow model. In Figure 6.9 we present the mean (bottom-middle) and the variance (bottom) of $F(\mu^y)$ characterised by posterior samples on the level set function mapped under F . In other words, these are the mean and variance from the κ 's obtained from the MCMC samples of the level / set function. As in the previous example, there is a critical value of $L = 0.3$ below of which the posterior estimates cannot accurately identify the main spatial features of κ^\dagger . Figure 6.10 shows posterior samples of the level set function (first, third and fifth rows) and the corresponding κ (second, fourth and sixth rows). The posterior samples, for values of L above the critical value $L = 0.3$, capture the main spatial features from the truth. There is, however, substantial uncertainty in the location of the interfaces. Our results offer evidence that this uncertainty can be properly captured with our level set Bayesian framework. Statistical measures of $F^* \mu^y$ (i.e. the posterior permeability measure on κ) is essential in practice. The proper quantification of the uncertainty in the unknown geologic facies is vital for the proper assessment of the environmental impact in applications such as CO₂ capture and storage, nuclear waste disposal and enhanced oil recovery.

In Figure 6.7 (bottom-right) we show the ACF of the first KL mode of level set function from different MCMC chains corresponding to different priors defined by the choices of L indicated previously. In contrast to the previous example, here we cannot appreciate substantial differences in the efficiency of the chain with respect to the selected values of L . However, we note that ACF exhibits a slow decay and thus long chains and/or multiple chains are need to properly explore the posterior. For the choice of $L = 0.4$ we consider 50 multiple MCMC chains. Our MCMC chains pass the Gelman-Rubin test [32] as we can note from Figure 6.7 (bottom-left) where we show the PSRF computed from MCMC samples of the level set function u (red-solid line) and the corresponding mapping, under the level set map, into the permeabilities κ (blue-dotted line). As indicated earlier, we may potentially increase the number of multiple chains and thus the number of uncorrelated samples form the posterior.

Figure 6.11 shows the prior and posterior densities of the first DCT coefficients on the κ obtained from the MCMC samples of the level set function (the vertical dotted line

corresponds to the DCT coefficient of the truth κ^\dagger). For some of these modes we clearly see that the posterior is concentrated around the truth. However, for the mode $\xi_{4,4}$ we note that the posterior is quite close to the prior indicating that the data have not informed this mode in any significant way.

Finally, in Figure 6.12 we display relative errors $\mathcal{E}_{L^1}(F(\bar{u}_n))$ (left), $\mathcal{E}_{L^1}(\bar{\kappa}_n)$ (middle) and $\mathcal{E}_{L^1}(F(u_n))$ (right) with \mathcal{E}_{L^1} as defined in (6.22). Accurate approximations are found for $L = 0.3, 0.35, 0.4$. As in Figure 6.6, the larger size of the errors in the rightmost panel is a reflection of the uncertainty in the reconstruction, and the posterior variance in the estimates.

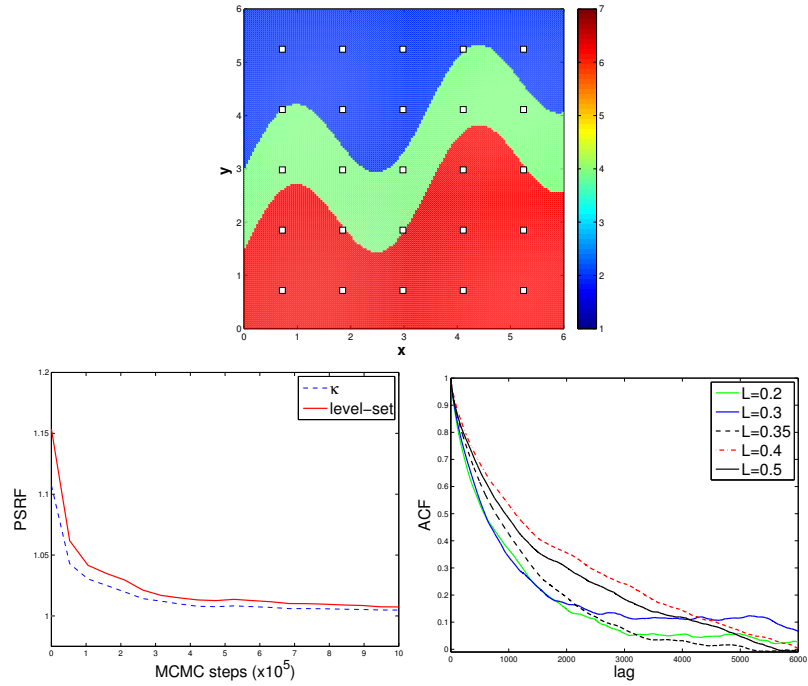


Figure 6.7: Identification of structural geology (channel model). Top: True κ in eq. (6.20). Bottom-left: PSRF from multiple chains with $L = 0.4$ in (6.15). Bottom-right: ACF of first KL mode of the level set function from single-chain MCMC with different choices of L .

6.4.5 Structural Geology: Layer Model

In this experiment we consider the groundwater model (6.20) with the same domain and measurement configurations from the preceding subsection. However, for this case we define the true permeability κ^\dagger displayed in Figure 6.13 (top). The permeability values are as before. The generation of synthetic data is conducted as described in the preceding subsection. For this example we consider the Gaussian prior on the level set defined by

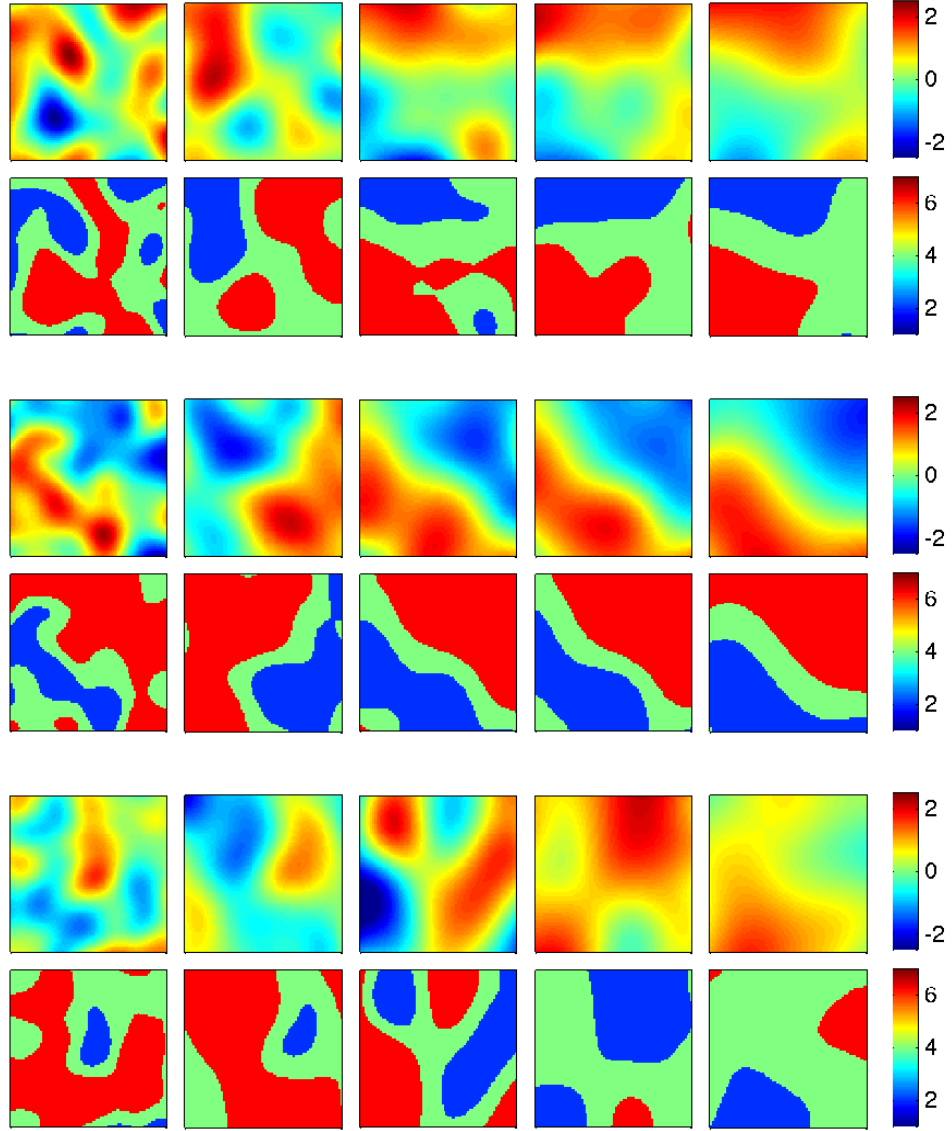


Figure 6.8: Identification of structural geology (channel model). Samples from the prior on the level set (first, third and fifth rows) for (from left to right) $L = 0.2, 0.3, 0.35, 0.4, 0.5$. push-forward onto κ (second, fourth and sixth rows) associated to each of these samples from the level set function.

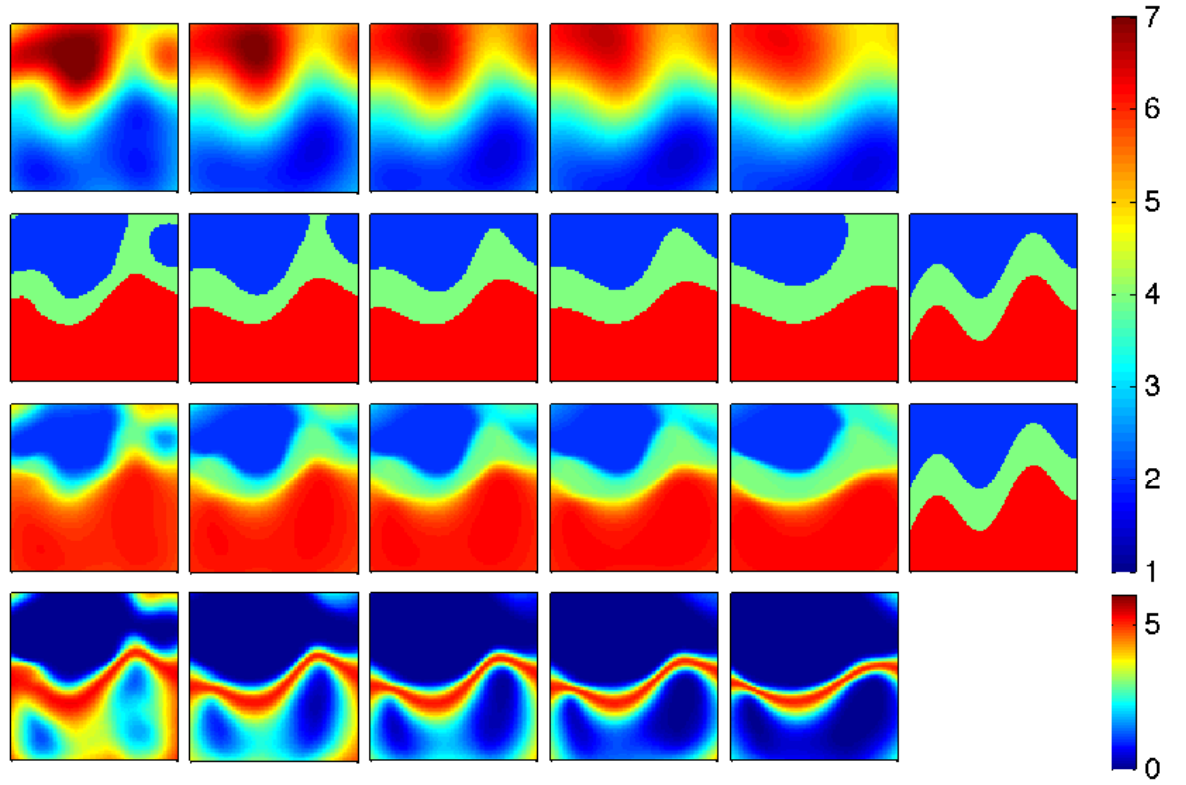


Figure 6.9: Identification of structural geology (channel model). MCMC results for (from left to right) $L = 0.2, 0.3, 0.35, 0.4, 0.5$ in the eq. (6.15). Top: MCMC mean of the level set function. Top-middle: κ associated to the mean of the level set function (true κ is displayed in the last column). Bottom-middle: Mean of the κ . Bottom: Variance of κ

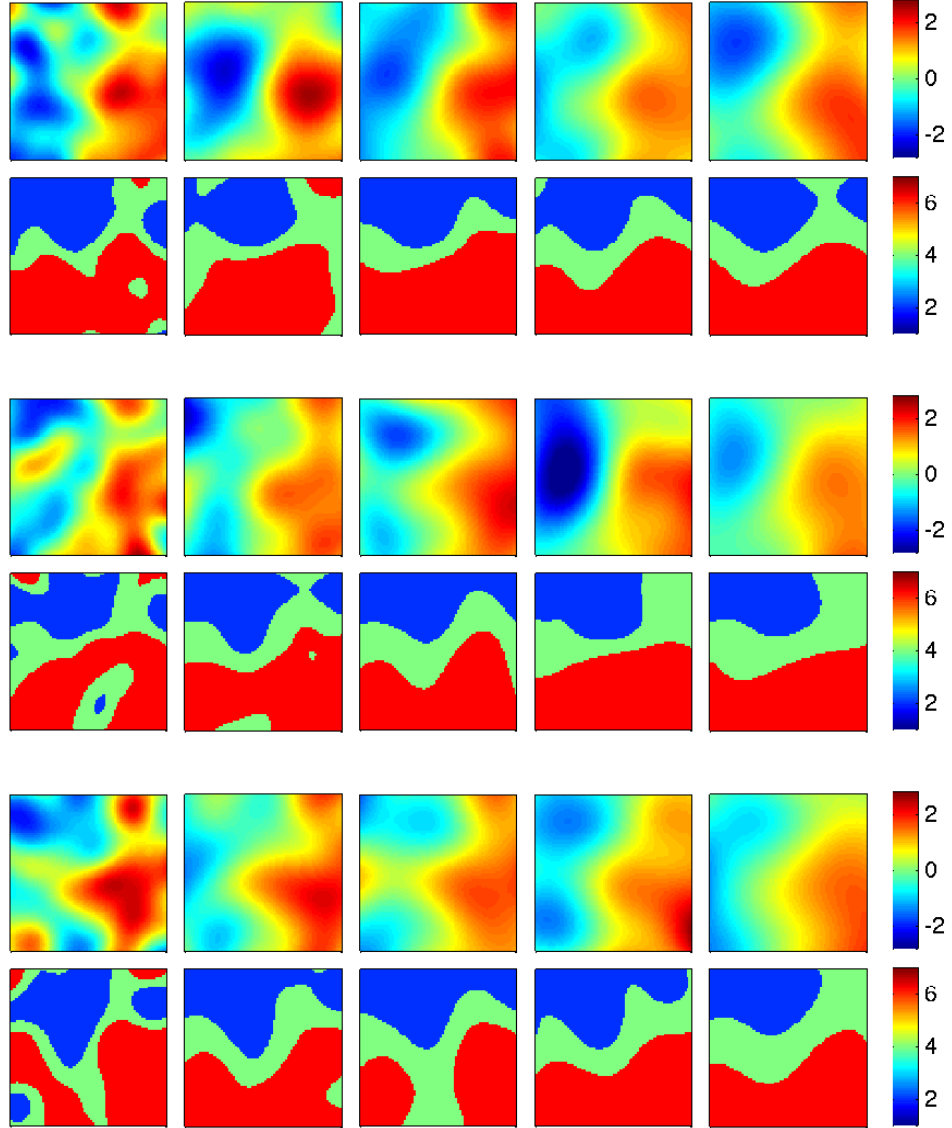


Figure 6.10: Identification of structural geology (channel model). Samples from the posterior on the level set (first, third and fifth rows) for (from left to right) $L = 0.2, 0.3, 0.35, 0.4, 0.5$. $\log(\kappa)$ (second, fourth and sixth rows) associated to each of these samples from the level set function.

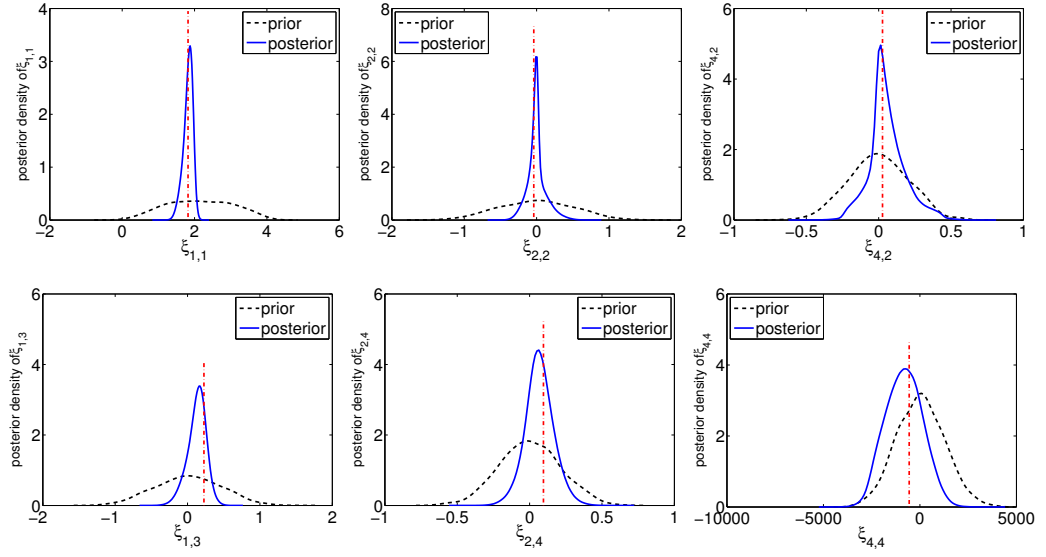


Figure 6.11: Identification of structural geology (channel model). Densities of the prior and posterior of some DCT coefficients of the κ 's obtained from MCMC samples on the level set for $L = 0.4$ (vertical dotted line indicates the truth).

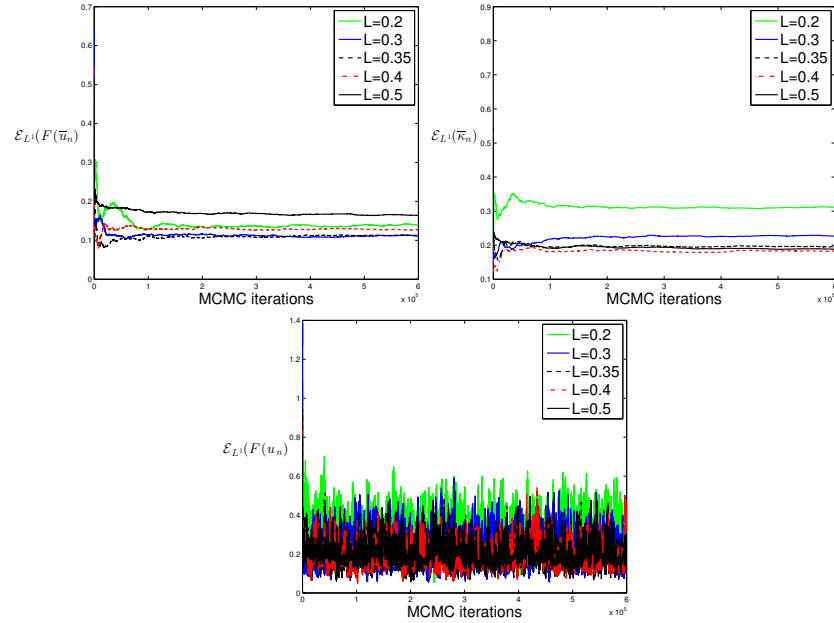


Figure 6.12: Identification of structural geology (channel model). $L^1(D)$ relative errors with respect to the truth for different choices of L . Left: $\mathcal{E}_{L^1}(F(\bar{u}_n))$. Middle: $\mathcal{E}_{L^1}(\bar{\kappa}_n)$. Right: $\mathcal{E}_{L^1}(F(u_n))$

(6.15). Since for this case the operator \mathcal{C} is diagonalisable by cosine functions, we use the fast Fourier transform to sample from the corresponding Gaussian measure $N(0, \mathcal{C})$ required by the pCN-MCMC algorithm.

The tunable parameter α in the covariance operator (6.15) determines the regularity of the corresponding samples of the Gaussian prior (see for example [215]). Indeed, in Figure 6.14 we show samples from the prior on the level set function (first, third and fifth rows) and the corresponding κ (second, fourth and sixth rows) for (from left to right) $\alpha = 1.5, 2.0, 2.5, 3.0, 3.5$. Indeed, changes in α have a dramatic effect on the regularity of the interface between the different regions. We therefore expect strong effect on the resulting posterior on the level set and thus on the permeability.

In Figure 6.15 we display numerical results from MCMC chains with different priors corresponding to (from left to right) $\alpha = 1.5, 2.0, 2.5, 3.0, 3.5$. In Figure 6.15 we present the MCMC mean of the level set function. The corresponding κ is shown in the top-middle of Figure 6.15. In this figure we additionally display the mean (bottom-middle) and the variance (bottom) of the κ 's obtained from the MCMC samples of the level set function. Above a critical value $\alpha = 2.5$ we obtain a reasonable identification of the layer permeability with a small uncertainty (quantified by the variance). Figure 6.16 shows posterior (MCMC) samples of the level set function (first, third and fifth rows) and the corresponding κ (second, fourth and sixth rows) for the aforementioned choices of α .

Figure 6.13 (bottom-right) shows the ACF of the first KL mode of level set function from MCMC experiments with different priors with α 's as before. The efficiency of the MCMC chain does not seem to vary significantly for the values above the critical value of α . However, as in the previous examples a slow decay in the ACF is obtained. An experiment using 50 multiple MCMC chains initialized randomly from the prior reveals that the Gelman-Rubin diagnostic test [32] is passed for $\alpha = 2.5$ as we can observe from Figure 6.13 (bottom-left) where we display PSRF from MCMC samples of the level set function (red-solid line) and the corresponding mapping into the κ (blue-dotted line). In Figure 6.17 we show the prior and posterior densities of the DCT coefficients on the κ obtained from the MCMC samples of the level set function (the vertical dotted line corresponds to the truth DCT coefficient). We see clearly that the DCT coefficients are substantially informed by the data although the spread around the truth confirms the variability in the location of the interface between the layers that we can ascertain from the posterior samples (see Figure 6.16).

In Figure 6.18 we present the relative errors with respect to the truth $\mathcal{E}_{L^1}(F(\bar{u}_n))$ (left), $\mathcal{E}_{L^1}(\bar{\kappa}_n)$ (middle) and $\mathcal{E}_{L^1}(F(u_n))$ (right). We note that $\alpha = 3.5$ provides the most accurate approximation of the truth. As in Figure 6.6, the larger size of the errors in the rightmost panel is a reflection of the uncertainty in the reconstruction, and the posterior

variance in the estimates.

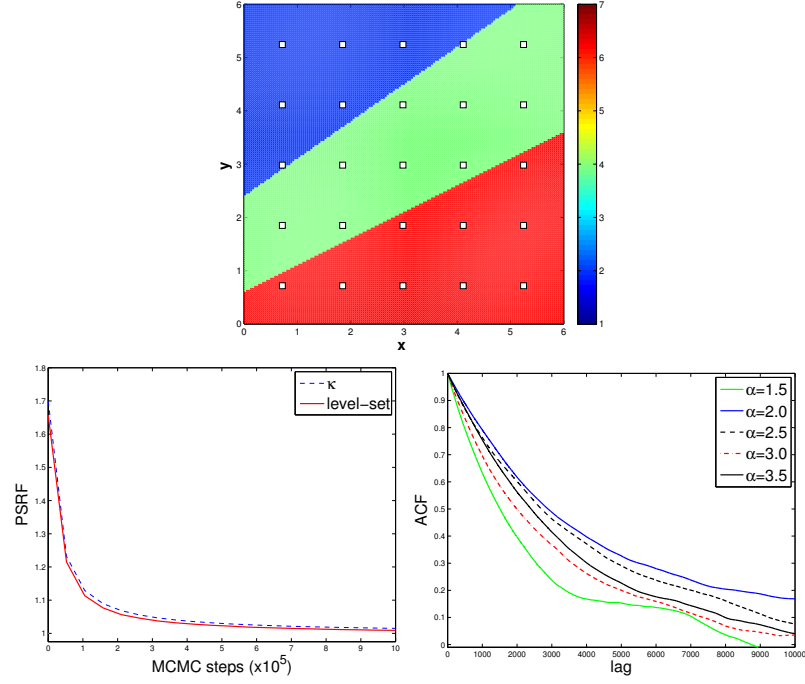


Figure 6.13: Identification of structural geology (layer model). Top: True κ in eq. (6.20). Bottom-left: PSRF from multiple chains with $\alpha = 2.5$ in (6.16). Bottom-right: ACF of first KL mode of the level set function from single-chain MCMC with different choices of α .

6.5 Conclusions

The primary contributions of this chapter are:

- We have formulated inverse problems for interfaces, within the Bayesian framework, using a level set approach.
- This framework leads to a well-posedness of the level set approach, something that is hard to obtain in the context of classical regularisation techniques for level set inversion of interfaces.
- The framework also leads to the use of state-of-the-art function-space MCMC methods for sampling of the posterior distribution on the level set function. An explicit motion law for the interfaces is not needed: the MCMC accept-reject mechanism implicitly moves them.

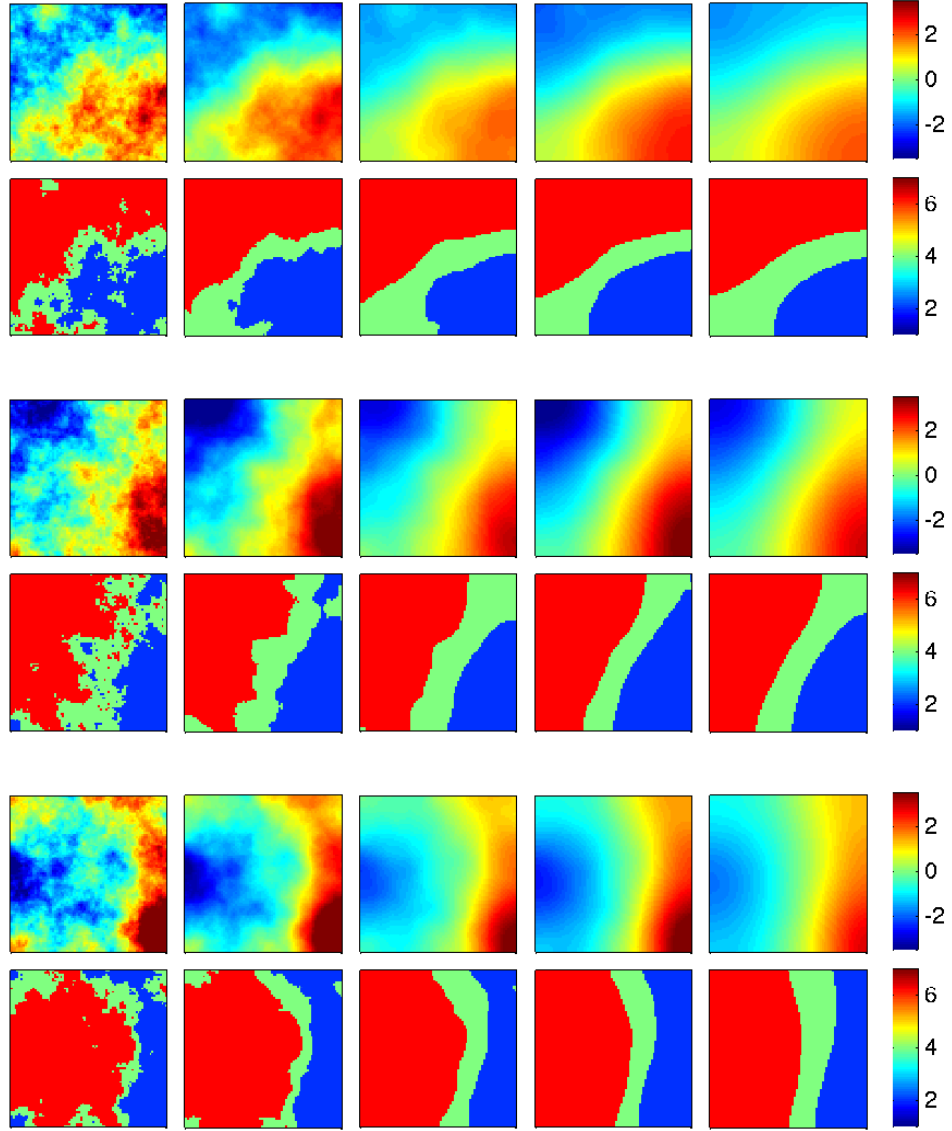


Figure 6.14: Identification of structural geology (layer model). Samples from the prior on the level set (first, third and fifth rows) for (from left to right) $\alpha = 1.5, 2.0, 2.5, 3.0, 3.5$ in (6.16). κ (second, fourth and sixth rows) associated to each of these samples from the level set function.

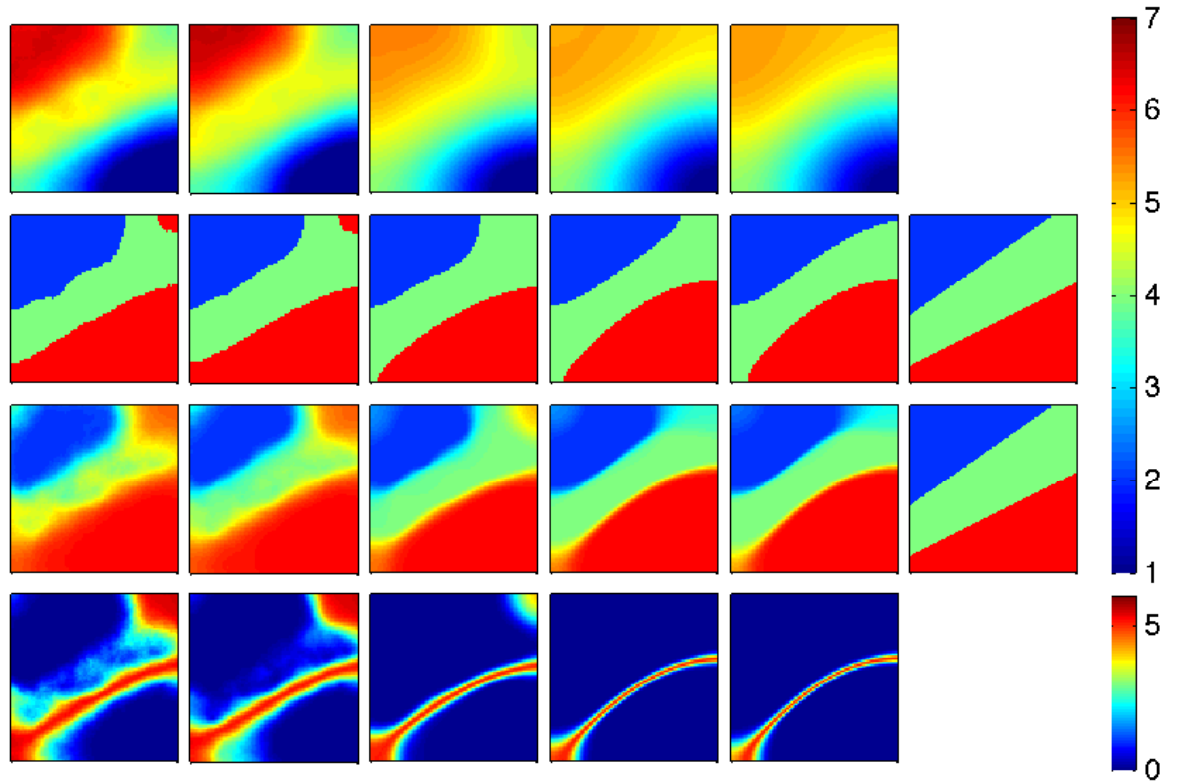


Figure 6.15: Identification of structural geology (layer model). MCMC results for (from left to right) $\alpha = 1.5, 2.0, 2.5, 3.0, 3.5$ in the eq. (6.16). Top: MCMC mean of the level set function. Top-middle: κ associated to the mean of the level set function (true κ is displayed in the last column). Bottom-middle: Mean of the κ . Bottom: Variance of κ

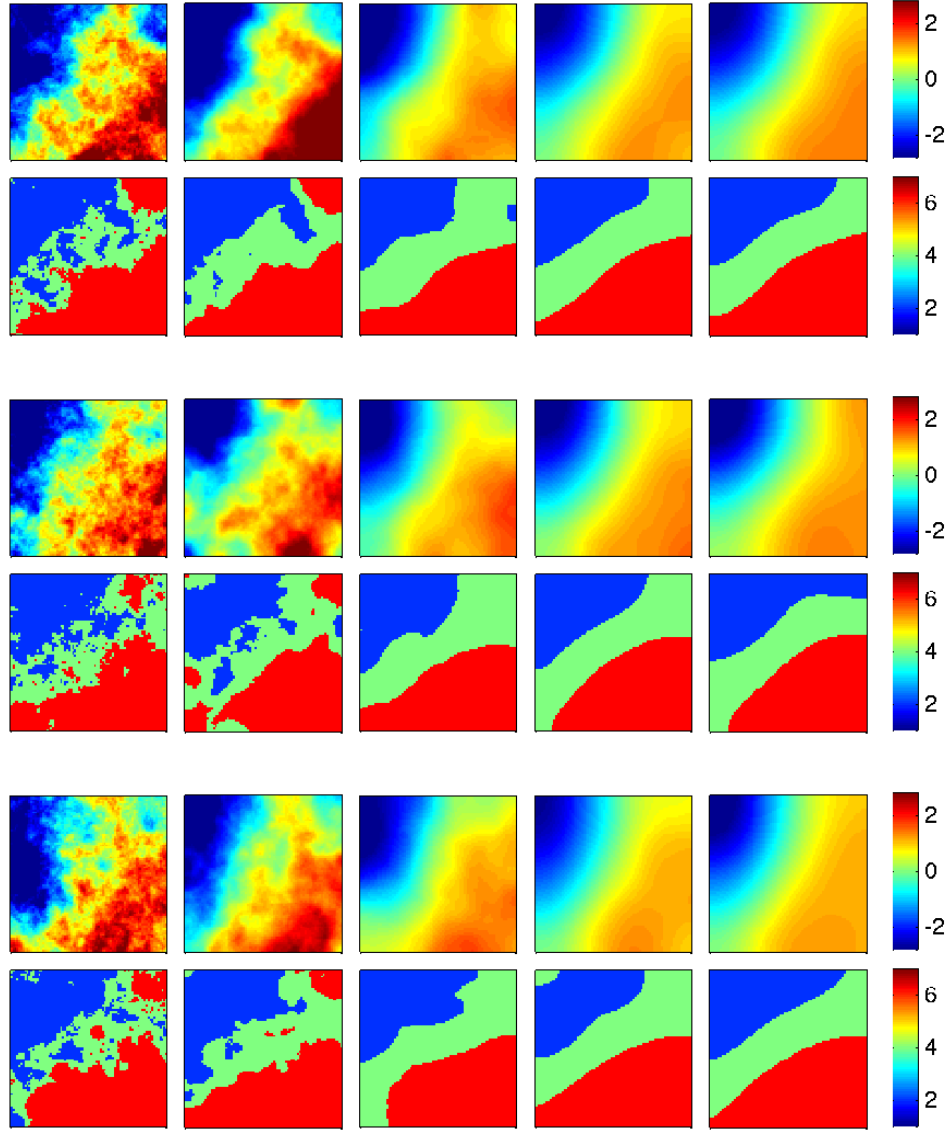


Figure 6.16: Identification of structural geology (layer model). Samples from the posterior on the level set (first, third and fifth rows) for (from left to right) $\alpha = 1.5, 2.0, 2.5, 3.0, 3.5$ in the eq. (6.16). κ (second, fourth and sixth rows) associated to each of these samples from the level set function.

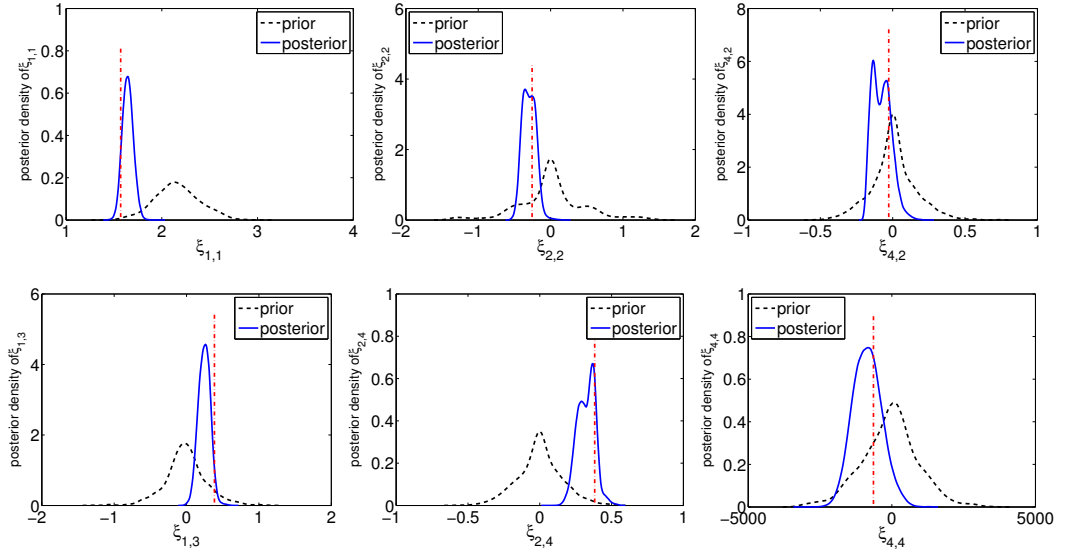


Figure 6.17: Identification of structural geology (layer model). Densities of the prior and posterior of some DCT coefficients of the κ 's obtained from MCMC samples on the level set for $L = 0.4$ (vertical dotted line indicates the truth).

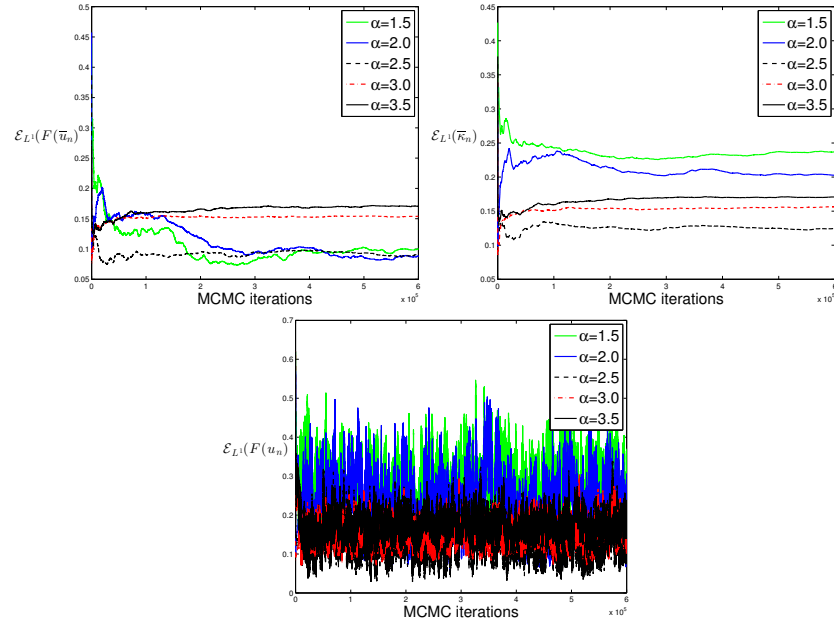


Figure 6.18: Identification of structural geology (layer model). $L^1(D)$ relative errors with respect to the truth for different choices of α in (6.16). Left: $\mathcal{E}_{L^1}(F(\bar{u}_n))$. Middle: $\mathcal{E}_{L^1}(\bar{\kappa}_n)$. Right: $\mathcal{E}_{L^1}(F(u_n))$

- We have studied two examples: inverse source reconstruction and an inverse conductivity problem. In both cases we have demonstrated that, with appropriate choice of priors, the abstract theory applies. We have also highlighted the behavior of the algorithms when applied to these problems.
- The fact that no explicit level set equation is required helps to reduce potential issues arising in level set inversion, such as reinitialisation. In most computational level set approaches [37], the motion of the interface by means of the standard level set equation often produces level set functions that are quite flat. For the mean curvature flow problem, such flattening phenomena was observed early in the history of level set evolution in [91] where the surface evolution starts from a “figure eight” shaped initial surface; in addition it has been shown to happen even if the initial surface is smooth [6]. This causes stagnation as the interface then moves slowly. Ad-hoc approaches, such as redistancing/reinitialising the level set function with a signed distance function, are then employed to restore the motion of the interface. In the proposed computational framework, not only does the MCMC accept-reject mechanism induce the motion of the interface, but it does so in a way that avoids creating flat level set functions underlying the permeability. Indeed, we note that the posterior samples of the level set function inherit the same properties from the ones of the prior. In particular, the probability of obtaining a level set function which takes any given value on a set of positive measure is zero under the posterior, as it is under the prior. This fact promotes very desirable, and automatic, algorithmic robustness.

Natural directions for future research include the following:

- The numerical results for the two examples that we consider demonstrate the sensitive dependence of the posterior distribution on the length-scale parameter of our Gaussian priors. It would be natural to study automatic selection techniques for this parameter, including hierarchical Bayesian modelling.
- We have assumed that the values of κ_i on each unknown domain D_i are both known and constant. It would be interesting, and possible, to relax either or both of these assumptions, as was done in the finite geometric parameterisations considered in [127].
- The numerical results also indicate that initialisation of the MCMC method for the level set function can have significant impact on the performance of the inversion technique; it would be interesting to study this issue more systematically.
- The level set formulation we use here, with a single level set function and possibly multiple level set values c_i has been used for modelling island dynamics [167] where

a nested structure is assumed for the regions $\{D_i\}_{i=1}^n$ see Figure 6.19(a). However, we comment that there exist objects with non-nested regions, such as those depicted in Figure 6.19(b)-6.19(c), which can not be represented by a single level set function. It would be of interest to extend this work to the consideration of vector-valued level set functions. In the case of binary obstacles, it is enough to represent the shape via a single level set function (cf. [204]). However, in the case of n -ary obstacles or even more complex geometric objects, the representation is more complicated; see the review papers [70, 71, 218] for more details.

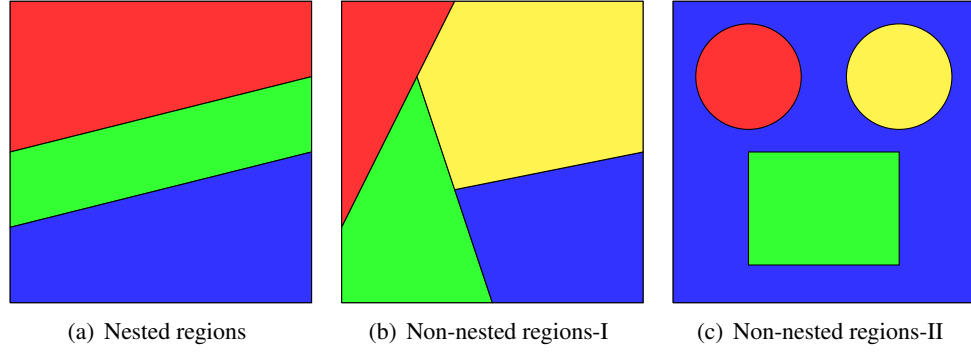


Figure 6.19: Nested regions and non-nested regions

- The Bayesian framework could be potentially combined with other parametrisations of unknown geometries. For example, the pluri Gaussian approach has been used with EnKF in [153] to identify geologic facies.

6.6 Appendix

6.6.1 Appendix 1

Proof of Theorem 6.2.3. Notice that the random variable $y|u$ is distributed according to the measure \mathbb{Q}_u , which is the translate of \mathbb{Q}_0 by $\mathcal{G}(u)$, satisfying $\mathbb{Q}_u \ll \mathbb{Q}_0$ with Radon-Nikodym derivative

$$\frac{d\mathbb{Q}_u}{d\mathbb{Q}_0}(y) \propto \exp\left(-\Phi(u; y)\right),$$

where $\Phi : U \times \mathbf{R}^J \rightarrow \mathbf{R}$ is the least squares function given in (6.9). Thus for the given data y , $\Phi(u; y)$ is up to a constant, the *negative log likelihood*. We denote by ν_0 the product measure

$$\nu_0(du, dy) = \mu_0(du)\mathbb{Q}_0(dy). \quad (6.23)$$

Suppose that $\Phi(\cdot, \cdot)$ is ν_0 measurable, then the random variable $(u, y) \in U \times Y$ is distributed according to $\nu(du, dy)$ with

$$\frac{d\nu}{d\nu_0}(u, y) \propto \exp(-\Phi(u; y)).$$

From Assumptions 6.2.2(2) and the continuity of $\Phi(u; y)$ with respect to y , we know that $\Phi(\cdot; \cdot) : U \times Y \rightarrow \mathbf{R}$ is continuous ν_0 -almost surely. Then it follows from Lemma 6.6.1 below that $\Phi(\cdot; \cdot)$ is ν_0 -measurable. On the other hand, by Assumptions 6.2.2(1), for $|y|_\Gamma \leq r$, we obtain the upper and lower bound for Z ,

$$0 < \exp(-K(r, \kappa_{\min})) \leq Z = \int_U \exp(-\Phi(u; y)) \mu_0(du) \leq 1.$$

Thus the measure is normalisable and applying the Bayes' Theorem 3.4 from [61] yields the existence of μ^y .

Let $Z = Z(y)$ and $Z' = Z(y')$ be the normalisation constants for μ^y and $\mu^{y'}$, i.e.

$$Z = \int_U \exp(-\Phi(u; y)) \mu_0(du), \quad Z' = \int_U \exp(-\Phi(u; y')) \mu_0(du).$$

We have seen above that

$$1 \geq Z, Z' \geq \exp(-K(r, \kappa_{\min})) > 0.$$

From Assumptions 6.2.2(3),

$$\begin{aligned} |Z - Z'| &\leq \int |\exp(-\Phi(u; y)) - \exp(-\Phi(u; y'))| \mu_0(du) \\ &\leq \int |\Phi(u; y) - \Phi(u; y')| \mu_0(du) \leq C(r) |y - y'|_\Gamma \end{aligned}$$

Thus, by the definition of Hellinger distance, we have

$$\begin{aligned} 2d_{\text{Hell}}(\mu^y, \mu^{y'})^2 &= \int \left(Z^{-1/2} \exp\left(-\frac{1}{2}\Phi(u; y)\right) - (Z')^{-1/2} \exp\left(-\frac{1}{2}\Phi(u; y')\right) \right)^2 \mu_0(du). \\ &\leq I_1 + I_2, \end{aligned}$$

where

$$\begin{aligned} I_1 &= \frac{2}{Z} \int \left(\exp\left(-\frac{1}{2}\Phi(u; y)\right) - \exp\left(-\frac{1}{2}\Phi(u; y')\right) \right)^2 \mu_0(du) \\ I_2 &= 2|Z^{-1/2} - (Z')^{-1/2}|^2 \int \exp(-\Phi(u; y')) \mu_0(du) \end{aligned}$$

Applying (1) and (2) in Assumptions 6.2.2 again yields

$$\frac{Z}{2}I_1 \leq C(r)|y - y'|_{\Gamma}^2$$

and

$$I_2 \leq C(r)|Z^{-1/2} - (Z')^{-1/2}|^2 \leq C(r)(Z^{-3} \vee (Z')^{-3})|Z - Z'|^2 \leq C(r)|y - y'|_{\Gamma}^2.$$

Therefore the proof that the measure is Lipschitz is completed by combining the preceding estimates. The final statement follows as in [215], after noting that $f \in L_{\mu_0}^2(U; S)$ implies that $f \in L_{\mu_y}^2(U; S)$, since $\Phi(\cdot; y) \geq 0$. \square

Lemma 6.6.1. *Let U be a separable Banach space and (U, Σ, μ) be a complete probability space with σ -algebra Σ . If a functional $\mathcal{F} : U \rightarrow \mathbf{R}$ is continuous μ -almost surely, i.e. $\mu(M) = 1$ where M denotes the set of the continuity points of \mathcal{F} , then \mathcal{F} is Σ -measurable.*

Proof. By the definition of measurability, it suffices to show that for any $c > 0$

$$S := \{u \in U \mid \mathcal{F}(u) > c\} \in \Sigma.$$

One can write S as $S = (S \cap M) \cup (S \setminus M)$. Since \mathcal{F} is continuous μ -almost surely, M is measurable and $\mu(M) = 1$. It follows from the completeness of the measure μ that $S \setminus M$ is measurable and $\mu(S \setminus M) = 0$. Now we claim that $S \cap M$ is also measurable. Denote $B_{\delta}(u) \subset U$ to be the ball of radius δ centred at $u \in U$. For each $v \in S \cap M$, as \mathcal{F} is continuous at v , there exists $\delta_v > 0$ such that if $v' \in B_{\delta_v}(v)$, then $\mathcal{F}(v') > c$. Therefore $S \cap M$ can be written as

$$S \cap M = M \bigcap \bigcup_{v \in S \cap M} B_{\delta_v}(v)$$

that is the intersection of the measurable set M with the open set $\bigcup_{v \in S \cap M} B_{\delta_v}(v)$. So $S \cap M$ is measurable. Then it follows that \mathcal{F} is Σ -measurable. \square

6.6.2 Appendix 2

Recall the Gaussian measure $\mu_0 = N(0, \mathcal{C})$ on the function space \mathcal{H} where $\mathcal{C} = \mathcal{C}_i$, $\mathcal{H} = \mathcal{H}_i$, $i = 1, 2$ given in Section 6.2.5. These measures can be constructed as Gaussian random fields.

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a complete probability space, i.e. if $A \in \mathcal{F}$ with $\mathbb{P}(A) = 0$, then $\mathbb{P}(B) = 0$ for $B \subset A$. A random field on D is a measurable mapping $u : D \times \Omega \rightarrow \mathbf{R}$. Thus, for any $x \in D$, $u(x; \cdot)$ is a random variable in \mathbf{R} ; whilst for any $\omega \in \Omega$, $u(\cdot; \omega) :$

$D \rightarrow \mathbf{R}$ is a vector field. Denote by $(\mathbf{R}^{\mathbb{N}}, \mathcal{B}(\mathbf{R}^{\mathbb{N}}), \mathbb{P})$ the probability space of i.i.d standard Gaussian sequences equipped with product σ -algebra and product measure. In this chapter, we consider $(\Omega, \mathcal{F}, \mathbb{P})$ as the completion of $(\mathbf{R}^{\mathbb{N}}, \mathcal{B}(\mathbf{R}^{\mathbb{N}}), \mathbb{P})$ in which case the σ -algebra \mathcal{F} consists of all sets of the type $A \cup B$, where $A \in \mathcal{B}(\mathbf{R}^{\mathbb{N}})$ and $B \subset N \in \mathcal{B}(\mathbf{R}^{\mathbb{N}})$ with $\mathbb{P}(N) = 0$. Let $\omega = \{\xi_k\}_{k=1}^{\infty} \in \Omega = \mathbf{R}^{\mathbb{N}}$ be an i.i.d sequence with $\xi_1 \sim N(0, 1)$, and consider the random function $u \in \mathcal{H}$ defined via the Karhunen-Loéve expansion

$$u(x; \omega) = \mathcal{T}(\omega) := \sum_{k=1}^{\infty} \sqrt{\lambda_k} \xi_k \phi_k(x), \quad (6.24)$$

where $\{\lambda_k, \phi_k\}_{k=1}^{\infty}$ is the eigensystem of \mathcal{C} . By the theory of Karhunen-Loéve expansions [21], the law of the random function u is identical to μ_0 . Recalling that $\alpha > 1$, the eigenvalues $\{\lambda_k\}$ of \mathcal{C}_1 decay like $k^{-\alpha}$ in two dimensions; whilst the eigenvalues of \mathcal{C}_2 will decay exponentially. Moreover, we assume further that $\phi_k \in U$ and that $\sup_k \|\phi_k\|_{\infty} < \infty$ which holds in simple geometries. Due to the decaying properties of the eigenvalues of \mathcal{C} , the truncated sum

$$\mathcal{T}_N(\omega) = \sum_{k=1}^N \sqrt{\lambda_k} \xi_k \phi_k \quad (6.25)$$

admits a limit \mathcal{T} in $L^2_{\mathbb{P}}(\Omega; \mathcal{H})$. By the Kolmogorov Continuity Theorem [61], \mathcal{T} is in fact Hölder continuous \mathbb{P} -almost surely; in particular, $\mathcal{T} \in U$ \mathbb{P} -almost surely. Then by Theorem 3.1.2 in [1], we have $\mathcal{T}_N \rightarrow \mathcal{T}$ in the uniform norm of U , \mathbb{P} -almost surely. Since for any $N \in \mathbb{N}$, $\mathcal{T}_N : (\Omega, \mathcal{F}) \rightarrow (U, \mathcal{B}(U))$ is continuous and thus measurable, we know from the completeness of $(\Omega, \mathcal{F}, \mathbb{P})$ that the limit \mathcal{T} is also measurable from (Ω, \mathcal{F}) to $(U, \mathcal{B}(U))$ (see p30 in [213]). The measurability of \mathcal{T} enables us to define a new measure on $(U, \mathcal{B}(U))$ which we still denote by μ_0 by the following:

$$\mu_0(A) = \mathbb{P}(\mathcal{T}^{-1}(A)) = \mathbb{P}(\{\omega \in \Omega \mid u(\cdot; \omega) \in A\}) \quad \text{for } A \in \mathcal{B}(U). \quad (6.26)$$

Thus μ_0 is indeed the push-forward measure of \mathbb{P} through \mathcal{T} . By definition, it is not hard to verify that μ_0 is the Gaussian measure $N(0, \mathcal{C})$ on $(U, \mathcal{B}(U))$. In addition, suppose that $B \subset N \in \mathcal{B}(U)$ with $\mu_0(N) = 0$; if we still define $\mu_0(B)$ according to (6.26), then $\mu_0(B) = \mathbb{P}(\mathcal{T}^{-1}(B)) = 0$ by the fact that $\mathcal{T}^{-1}(B) \subset \mathcal{T}^{-1}(N)$ and the completeness of $(\Omega, \mathcal{F}, \mathbb{P})$. Denote by Σ the smallest σ algebra containing $\mathcal{B}(U)$ and all sets of zero measure under μ_0 so that any set $E \in \Sigma$ is of the form $E = A \cup B$, where $A \in \mathcal{B}(U)$ and $B \subset N \in \mathcal{B}(U)$ with $\mu_0(N) = 0$. Then (U, Σ, μ_0) is complete.

We comment that although a Gaussian measure is usually defined as a Borel mea-

sure in the literature (see e.g. [21]), it is more convenient to work with a complete Gaussian measure in this chapter; in particular, the completeness of μ_0 is employed to show the measurability of the observational map in level set based inverse problems.

Considering a Gaussian random function $u(\cdot; \omega)$ with $\omega \in \Omega$, for any level constant $c \in \mathbf{R}$, we define the random level set

$$D_c^0 = D_c^0(u(\cdot; \omega)) = D_c^0(\omega) := \{x \mid u(x; \omega) = c\}. \quad (6.27)$$

Recall that the measure space (U, Σ, μ_0) is the push-forward of $(\Omega, \mathcal{F}, \mathbb{P})$ under \mathcal{T} . We define the functional $\mathcal{M}_c : U \rightarrow \mathbf{R}$ by

$$\mathcal{M}_c u = m(\{x \mid u(x) = c\})$$

and the composition $\mathcal{R}_c := \mathcal{M}_c \circ \mathcal{T}$, as illustrated in the following commutative diagram:

$$\begin{array}{ccc} (\Omega, \mathcal{F}, \mathbb{P}) & \xrightarrow{\mathcal{T}} & (U, \Sigma, \mu_0) \\ & \searrow \mathcal{R}_c = \mathcal{M}_c \circ \mathcal{T} & \downarrow \mathcal{M}_c \\ & & (\mathbf{R}, \mathcal{B}(\mathbf{R})) \end{array}$$

Lemma 6.6.2. *For any $c \in \mathbf{R}$, \mathcal{M}_c is Σ -measurable and \mathcal{R}_c is \mathcal{F} -measurable so that $m(D_c^0)$ is a random variable on both (U, Σ, μ_0) and $(\Omega, \mathcal{F}, \mathbb{P})$.*

Proof. To prove \mathcal{M}_c is Σ -measurable, we only need to check the set $A_t := \{u \in U \mid \mathcal{M}_c u \geq t\} \in \Sigma$ for any $t \in \mathbf{R}$. Since \mathcal{M}_c is a non-negative map, for $t \leq 0$, it is obvious that $A_t = U$ and hence measurable. Now we claim that A_t is closed in U for $t > 0$. To that end, let $\{u_n\}_{n=1}^\infty$ be a sequence of functions in A_t such that $\|u_n - u\|_U \rightarrow 0$ for some $u \in U$ as $n \rightarrow \infty$. We prove that $u \in A_t$. Since $\|u_n - u\|_U \rightarrow 0$, there exists a subsequence which is still denoted by u_n such that $\|u_n - u\|_U < 1/n$. By the definition of A_t , $u_n \in A_t$ means that $m(\{x \in \overline{D} \mid u_n(x) = c\}) \geq t$ for all n . Moreover, from the construction of u_n , $\{x \in \overline{D} \mid u_n(x) = c\} \subset B_n := \{x \in \overline{D} \mid |u(x) - c| < 1/n\}$, which implies that $m(B_n) \geq t$. Noting that

$$\{x \in \overline{D} \mid u(x) = c\} = \cap_{n=1}^\infty B_n$$

and that B_n is decreasing, we can conclude that $m(\{x \in \overline{D} \mid u(x) = c\}) \geq t$, i.e. $u \in A_t$. So A_t is closed for $t > 0$. Then it follows from the measurability of \mathcal{T} that \mathcal{R}_c is \mathcal{F} -measurable. Therefore $m(D_c^0)$ is a random variable on both (U, Σ, μ_0) and $(\Omega, \mathcal{F}, \mathbb{P})$. \square

The following theorem demonstrates that $m(D_c^0)$ vanishes almost surely on both

measure spaces above.

Proposition 6.6.3. *Consider a random function u drawn from one of the Gaussian probability measures μ_0 on (U, Σ) given in Section 6.2.5. For $c \in \mathbf{R}$, the random level set D_c^0 of u is defined by (6.27). Then*

- (i) $m(D_c^0) = 0, \mathbb{P}$ -almost surely;
- (ii) $m(D_c^0) = 0, \mu_0$ -almost surely.

Proof. (i) For any fixed $x \in D$, since the point evaluation $u(x)$ acts as a bounded linear functional on U , $u(x; \cdot)$ is a real valued Gaussian random variable, which implies $\mathbb{P}(\{\omega \mid u(x, \omega) = c\}) = 0$. Moreover, noting that the random field $u : D \times \Omega \rightarrow \mathbf{R}$ is a measurable map, if we view $m(D_c^0)$ as a random variable on Ω , then

$$\begin{aligned} \mathbb{E}[m(D_c^0)] &= \int_{\Omega} m(D_c^0(\omega)) \, d\mathbb{P}(\omega) = \int_{\Omega} \int_{\mathbf{R}^d} \mathbf{1}_{\{x \mid u(x; \omega) = c\}} \, dx \, d\mathbb{P}(\omega) \\ &= \int_{\Omega} \int_{\mathbf{R}^d} \mathbf{1}_{\{(x, \omega) \mid u(x; \omega) = c\}} \, dx \, d\mathbb{P}(\omega) \stackrel{\text{Fubini}}{=} \int_{\mathbf{R}^d} \int_{\Omega} \mathbf{1}_{\{(x, \omega) \mid u(x; \omega) = c\}} \, d\mathbb{P}(\omega) \, dx \\ &= \int_{\mathbf{R}^d} \int_{\Omega} \mathbf{1}_{\{\omega \mid u(x; \omega) = c\}} \, d\mathbb{P}(\omega) \, dx = \int_{\mathbf{R}^d} \mathbb{P}(\{\omega \mid u(x; \omega) = c\}) \, dx = 0. \end{aligned}$$

Noting that $m(D_c^0) \geq 0$, we obtain $m(D_c^0) = 0, \mathbb{P}$ -almost surely.

(ii) Recall that $A_t = \{u \in U \mid \mathcal{M}_c u \geq t\}$ defined in Lemma 6.6.2 is closed in U for any $t > 0$. Thus the set $A := \{u \in U \mid m(\{x \mid u(x) = c\}) = 0\} = (\cup_{k=1}^{\infty} A_{1/k})^c = \cap_{k=1}^{\infty} A_{1/k}^c$ is a Borel set of U and measurable. Since μ_0 is the push-forward measure of \mathbb{P} under \mathcal{T} ,

$$\mu_0(A) = \mathbb{P}(\mathcal{T}^{-1}(A)) = \mathbb{P}(\{\omega \mid m(D_c^0(\omega)) = 0\}) = 1,$$

where the last equality follows from (i). □

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